

APPROVAL SHEET

Title of Thesis: Electrons and Spin Waves in Itinerant Ferromagnets

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ABSTRACT

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Though it is accepted that the 3-d magnetic electrons of transition metals such as nickel are itinerant, at high temperature these itinerant ferromagnets act as if the electrons were localized at lattice sites. In particular, three experimental results conflict with the Stoner itinerant model: 1) The spin band gap does not decrease with temperature as the average magnetization, but much more slowly. 2) Spin waves of short wavelength propagate above the Curie temperature. 3) Magnetic degrees of freedom play a role in determining thermodynamic properties near and above T_C . The source of these discrepancies is the failure of Stoner theory to take into account magnetization fluctuations. In this paper, I do calculations of single particle and spin wave properties in a generalization of Stoner theory devised by R. E. Prange and V. Korenman to take account of fluctuations.

In Stoner theory, electrons interact with an effective magnetic field proportional to the average magnetization, which becomes zero at the phase transition. The basic idea of the generalization of Stoner theory is that electrons are sensitive to their local environment and therefore that electronic and spin wave properties should be calculated in the presence of a local slowly fluctuating magnetization configuration. Only after calculating these properties should the fluctuations

be thermally averaged. As a result, electrons interact with an effective magnetic field which is basically proportional to the magnitude of the local magnetization vector and which need not become zero at T_c .

Single particle properties are calculated by making a transformation to the spatially varying frame of reference of the local magnetization and doing perturbation theory with the magnetization gradients as the small perturbation parameter. We find that the spin eigenstates are approximately in or opposite to the direction of the local magnetization. Even when there is no longer a macroscopic magnetization, an energy gap is maintained between spin-split bands, the bands now being defined in terms of the local magnetization direction. The change in the energy gap from its zero temperature value is proportional only to the average square of a magnetization gradient, a quantity which may be small even above T_c . Thus we can understand that the gap changes only slowly with temperature and that the spin wave does not decay into Stoner single particle excitations even at high temperature.

A free energy is found which is very similar in form to the free energy used to compute thermodynamic properties in localized models; thus we find that magnetic degrees of freedom are still important in computing thermodynamic properties above T_c .

It is the existence of a population difference and energy gap, rather than a macroscopic average magnetization that permits the existence of a spin flip collective excitation. We find a secular equation for the spin wave frequency in the presence of fluctuations

which is very similar to the usual RPA secular equation, except for small perturbations proportional to the square of magnetization gradients. The corrections to the spin wave frequency and lifetime include the effect of the perturbation of single electron energies by the background, and also of the scattering of the spin wave from single particle spin-conserving excitations and from other spin waves. These corrections are quite small and allow for propagation even above T_C . Thus it is a prediction of our theory that one see spin waves even above the critical temperature, so long as an appropriate population difference maintains a locally ordered magnetization.

ELECTRONS AND SPIN WAVES
IN ITINERANT FERROMAGNETS

by

Joanne L. Murray

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CHAPTER 1

STONER THEORY

In this paper I present calculations which describe the ferromagnetism of a system that is a good approximation to a transition metal like nickel.

Two kinds of model are available for the description of a ferromagnetic metal: in the Stoner picture, the magnetic electrons are itinerant and participate in the band structure of the metal; in models such as those of Heisenberg or Ising, the magnetic moments are localized at lattice sites. In a localized model, the phase transition consists in the ordering or disordering of permanent moments. In itinerant models, ferromagnetism occurs because bands of electrons with spin aligned parallel or anti-parallel to a net magnetic moment of the metal have different occupations; the phase transition consists in a reoccupation of the spin bands. Because the sources of the magnetic phase transition are different in the two kinds of model, the two models give rise to different magnetic and thermodynamic properties.

The problem encountered by any theory of transition metal ferromagnets is that they behave like itinerant ferromagnets at low temperature and like Heisenberg ferromagnets near the transition temperature; neither kind of theory is adequate for all temperatures. Localized models are inadequate simply because the magnetic electrons are indeed free to move through the crystal; but an itinerant model does not handle the magnetization fluctuations properly, especially at high temperatures. I have made calculations of single particle

and spin wave properties in a generalization of the Stoner theory devised by R. E. Prange and V. Korenman to account for magnetization fluctuations at both high and low temperatures.

In the first chapter, I shall review some results of the Stoner model and describe how that model goes wrong. I shall present some of the Stoner calculations in detail, because my own calculations are done by similar methods and have results similar in form. After giving a brief discussion of some recent attempts to cope with magnetization fluctuations, I shall describe the physical picture upon which my calculations are based.

II The Bands in Nickel

The 3-d magnetic electrons of transition metal ferromagnets are certainly not localized at lattice sites. They contribute to the low temperature specific heat and conductivity, and this means that they are free to move through the crystal in response to an external field. Moreover, they participate in the band structure and have a well-defined Fermi surface, which can be seen in the de Haas-van Alphen effect or in photoemission studies.

Though our results will be applicable to any itinerant ferromagnet, we shall always apply them to nickel, because the 3-d bands of nickel have properties which make them especially amenable to treatment in the approximation scheme we are going to use. The band structure of nickel has the following properties:

(1) The magnetic electrons belong to the XW region of the Brillouin zone. There the d-bands are split into two bands separated

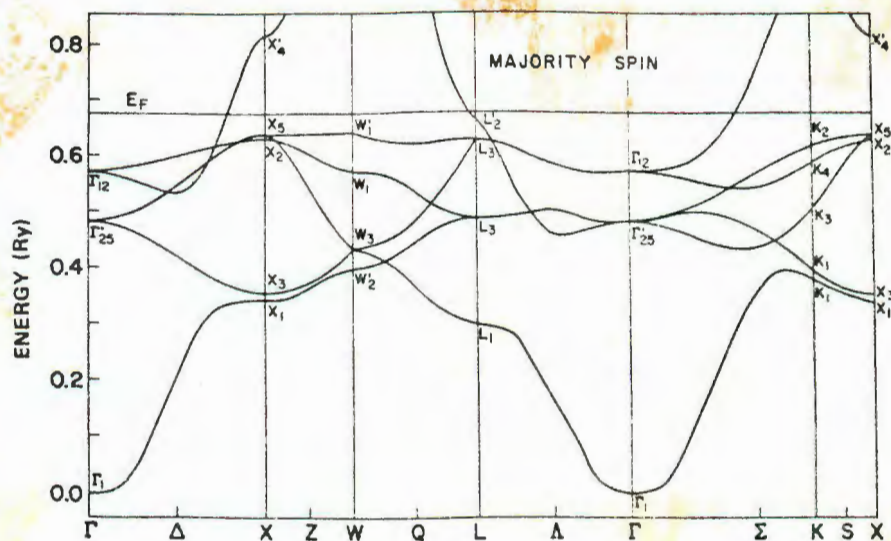


FIG. 1. Band structure for majority-spin states along certain symmetry directions. The horizontal line at 0.675 Ry indicates the position of the Fermi energy.

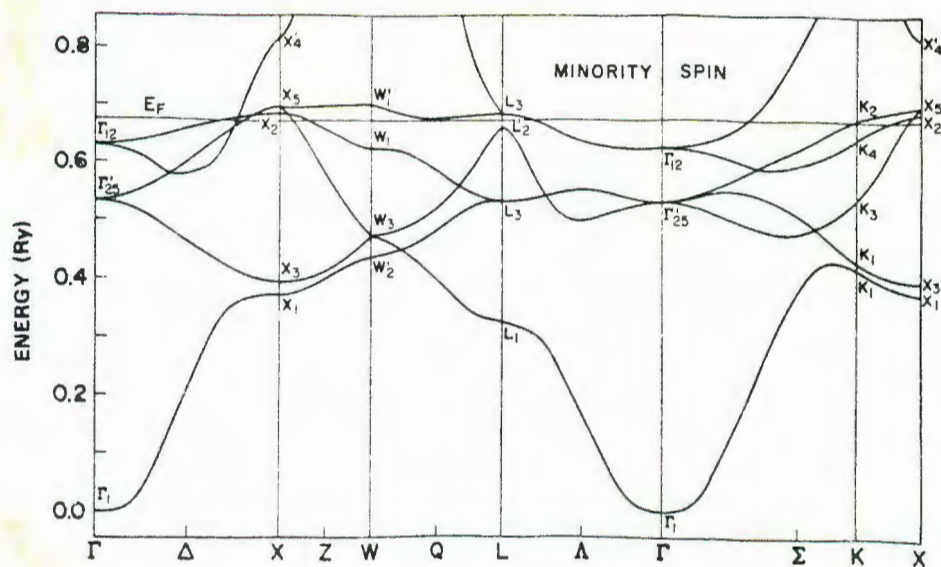


FIG. 2. Band structure for minority-spin states along certain symmetry directions.

Diagrams from Callaway and Wang^[1].

in energy by about 0.4 eV. The difference in population between the majority and minority bands is 0.6 electrons per atom. This is a low density of magnetic carriers compared to that of iron or cobalt, which have moments of 1.7 and 2.9 electrons/atom.

(2) The Fermi level is near the top of the majority spin band, so that the magnetic carriers can be thought of as holes in the minority spin band. For convenience we shall always consider the holes to be particles and speak of an empty minority spin band for nickel; when the energy gap is larger than the Fermi energy, as in this case, we are said to be in the strong limit.

(3) The 3-d bands are narrow and very flat in the XW region. One effect of this is that there is very little hybridization of d-bands with the sp bands. The velocity of s-electrons $k_F/m_s \gg k_F/m_d$, so that the s-electrons respond quickly to the motions of the d-electrons: to ignore the s-electrons is to make an adiabatic approximation. Hence we have well-defined d-bands which correspond to atomic d-orbitals. The flatness at the top of the band will also lead to a peak in the density of states near the Fermi level.

(4) The bands of interest are tight binding bands corresponding to the yz, xy, and zx orbitals; these tight binding bands do not mix at the point X because of the symmetry of the wave functions. Therefore there are three degenerate bands, one formed from each of the above d-orbitals.

Using these properties of the bands, Kanamori^[2] has shown that nickel can be represented by a one-band picture, with the following Hamiltonian of Hubbard form:

$$H = \sum_{\mathbf{k}\sigma} n(\mathbf{k},\sigma)\epsilon(\mathbf{k}) + U \sum_i n_{i\uparrow} n_{i\downarrow} ;$$

$n(\mathbf{k},\sigma)$ is the number operator of the Bloch state of wavevector \vec{k} and spin σ , $\epsilon(\mathbf{k})$ is the band energy, and $n_{i\sigma}$ is the number operator for the Wannier state centered at site i . U is an effective intra-atomic Coulomb energy and is approximately 1.5 eV.

III The Criterion for Ferromagnetism in Molecular Field Theory

It is useful to express the Coulomb exchange energy in terms of operators $a_{\mathbf{k}\sigma}^\dagger$ which create an electron of spin σ in a Bloch state of wavevector \vec{k} . The Hubbard Hamiltonian in this representation is

$$\sum_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} \epsilon(\mathbf{k}) + U \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} a_{\mathbf{k}+\mathbf{q}\uparrow}^\dagger a_{\mathbf{k}\uparrow} a_{\mathbf{k}'-\mathbf{q}\downarrow}^\dagger a_{\mathbf{k}'\downarrow} .$$

In the Hartree-Fock approximation, this provides effective single particle energies $\epsilon(\mathbf{k},\sigma) = \epsilon(\mathbf{k}) - \sigma n_{-\sigma} U$

or, shifting each by a constant energy, $\epsilon(\mathbf{k},\sigma) = \epsilon(\mathbf{k}) - \sigma \Delta/2$.

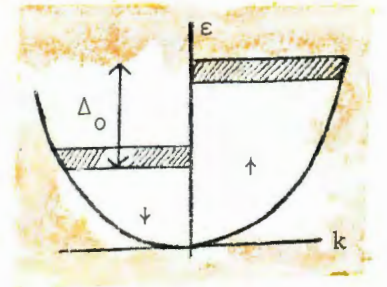
The band gap $\Delta = \epsilon(\mathbf{k}\downarrow) - \epsilon(\mathbf{k}\uparrow) = U(n_{\uparrow} - n_{\downarrow}) = MU$

represents the interaction of the spin with a Weiss mean field. The total magnetic energy is $\frac{1}{4} M^2 U = \frac{1}{4} M \Delta$; the extra factor of $\frac{1}{2}$ must be introduced so that interactions are not counted twice. Notice that Δ is proportional to M and thus vanishes at and above the Curie temperature.

We can find a criterion for ferromagnetism at zero temperature by requiring that near the paramagnetic state (that is, for a small gap and magnetization) the energy not be lowered by a decrease in the magnetization. If δn spins are flipped from \uparrow to \downarrow , the kinetic

energy change is $-\delta n \Delta$. The magnetic energy change is $\frac{1}{2} \delta M \Delta + \frac{1}{2} M \delta \Delta$;
and the change in the gap is

$$\delta \Delta = (1/N_{\uparrow} + 1/N_{\downarrow}) \delta n \sim 2 \delta n / N(\epsilon_F)$$



(N_{σ} is the density of states $dN/d\epsilon$ at the σ Fermi level.) Putting these together, we find the Stoner criterion for ferromagnetism to be that $UN(\epsilon_F) > 1$.

This is equivalent to requiring that the paramagnetic zero temperature susceptibility be negative or infinite. For small field, and hence small gap and magnetization, the magnetization is

$$\begin{aligned} M &= \int \{f(\epsilon - \mu H - \frac{1}{2} \mu U) - f(\epsilon + \mu H + \frac{1}{2} \mu U)\} N(\epsilon) d\epsilon \\ &= -(2\mu H + \mu U) \int \frac{df}{d\epsilon} N(\epsilon) d\epsilon \end{aligned}$$

with $f(\epsilon)$ the Fermi function $\{\exp(\beta\epsilon - \beta\mu) + 1\}^{-1}$.

Therefore we find a susceptibility

$$\chi \equiv \frac{dM}{dH} = \frac{2\mu N(\epsilon_F)}{1 - UN(\epsilon_F)}$$

which shows the divergence required above.

When the Stoner criterion is satisfied, the system spontaneously becomes ordered. The magnetization is determined by requiring simultaneously that

$$\begin{aligned} N &= \int d\epsilon N(\epsilon) \{f(\epsilon - \frac{1}{2} \mu U) + f(\epsilon + \frac{1}{2} \mu U)\} \\ M &= \int d\epsilon N(\epsilon) \{f(\epsilon - \frac{1}{2} \mu U) - f(\epsilon + \frac{1}{2} \mu U)\} \end{aligned}$$

The susceptibility is no longer given by the equation above and is finite and positive.

IV The Magnetization at Low Temperature

In the Stoner model at finite temperature, the magnetization is reduced from its zero temperature value by single particle excitations from the spin up to the spin down band. In a non-magnetic material, the chemical potential changes with temperature in order to keep the number of particles fixed. In a magnetic material, since the Fermi level occurs at different wavevectors in the two bands, the shifts in chemical potential are different. The chemical potentials, however, must be the same for both spin bands: there must be some redistribution of electrons between the bands to maintain this equality as the temperature increases.

The total shifts in the chemical potentials at low temperature are;

$$\delta\mu_{\uparrow,\downarrow} = -\frac{\pi^2}{6} \frac{dN/d\varepsilon}{N_{\uparrow,\downarrow}} (kT)^2 + \frac{\delta n_{\uparrow,\downarrow}}{N_{\uparrow,\downarrow}} \mp \frac{1}{2}\delta MU$$

The first term comes from the usual shift in the chemical potential at constant occupation, the second from the concomitant repopulation, and the last from the shift in the magnetic interaction energy caused by the repopulation. The repopulation can now be determined by requiring that $\delta\mu_{\uparrow} = \delta\mu_{\downarrow}$ and using the constraint that the total number of particles be fixed, $\delta n_{\uparrow} = -\delta n_{\downarrow}$. Then

$$\delta M = -(1/N_{\uparrow} + 1/N_{\downarrow} - 2U)^{-1} \frac{\pi^2}{3} (kT)^2 (N'_{\downarrow}/N_{\downarrow} - N'_{\uparrow}/N_{\uparrow}).$$

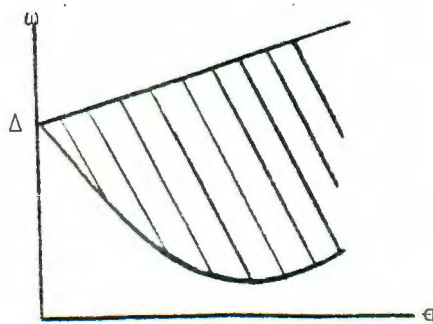
In the strong limit, repopulation is prevented by an energy gap $\Delta - \mu$ between the Fermi level and the lowest energy down-spin state. Repopulation occurs only because of the exponential high energy tail of the distribution function, and δM is proportional to $\exp(-(\Delta - \mu)/kT)$. These Stoner terms are seen in the temperature dependence of the

magnetization. However, there is a more important source of temperature dependence of the magnetization, and that is the spin waves. In both the weak and the strong cases, spin waves contribute a term

$$\delta M = \sum_q v(q) \cong T^{3/2}.$$

V Spin Waves

The only spin flip excitations which appear in Stoner theory are single particle excitations $a_{\downarrow}^{\dagger}(k+q) a_{\uparrow}(k) |\Phi_0\rangle$. ($|\Phi_0\rangle$ is the zero temperature ground state, and $a_{\downarrow}^{\dagger}(k+q) a_{\uparrow}(k)$ destroys an up electron of momentum \vec{k} and replaces it by a down electron of $\vec{k}+\vec{q}$.) These excitations have the large energy, $\hbar\omega = \epsilon(k+q) - \epsilon(k) + \Delta$; and they produce the following excitation spectrum:



To find a low energy collective excitation, we must treat the Hubbard Hamiltonian in some approximation better than molecular field theory.

We guess that a collective excitation can be formed by making a linear combination of Stoner excitations:

$$|q\rangle \equiv \sum_p c_p a_{\downarrow}^{\dagger}(p+q) a_{\uparrow}(p) |\Phi_0\rangle.$$

To find the coefficients c_p and the excitation energy, we minimize the expectation of the Hamiltonian and constrain the state to be normalized. If we minimize the quantity $\langle q | H | q \rangle - \omega \langle q | q \rangle$ with respect to each coefficient c_p , $\omega(q)$ will be the excitation energy.

If we do this in the molecular field approximation, we find the following equation for c_p :

$$c_p \{ \epsilon(p+q) - \epsilon(p) + \Delta - \hbar\omega \} = 0.$$

This gives us back the Stoner excitations.

If we use the full two-particle Hubbard interaction energy,

$$U \sum_{kk'\lambda} a_{\uparrow}^{\dagger}(k+\lambda) a_{\uparrow}(k) a_{\downarrow}^{\dagger}(k'-\lambda) a_{\downarrow}(k'), \text{ we find}$$

$$c_p \{ \epsilon(p+q) - \epsilon(p) + \Delta - \hbar\omega \} = U \sum_{p'} c_{p'},$$

which has solutions

$$c_p = \text{constant} \{ f_{\uparrow}(p) - f_{\downarrow}(p+q) \} \{ \epsilon(p+q) - \epsilon(p) + \Delta - \hbar\omega \}^{-1}$$

The secular equation determining ω is:

$$1 = U \sum_p \frac{f_{\uparrow}(p) - f_{\downarrow}(p+q)}{\epsilon(p+q) - \epsilon(p) + \Delta - \hbar\omega}$$

The solution of interest has small $|\vec{q}|$ ($qv_F \ll \Delta$) and energy ($\omega \ll \Delta$).

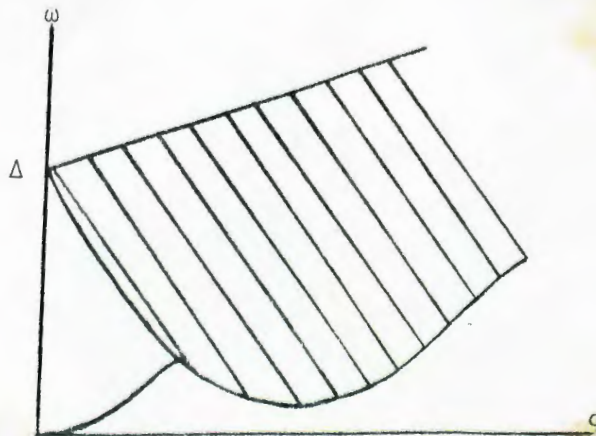
We can expand the denominator in powers of $1/\Delta$ to find

$$\hbar\omega = q^2 \left\{ \sum_{\text{all}} \frac{1}{2} \nabla^2 \epsilon - \sum_{\text{so}} (\nabla \epsilon_k)^2 / \Delta \right\} / 3M \equiv D q^2$$

The notation \sum_{all} means sum over all occupied states of both spins; \sum_{so}

means sum over the singly occupied states.

Apparently the stiffness is proportional to $1/M$, but in fact it is not large when M becomes small. To see the magnetization dependence of the stiffness of a weak ferromagnet, we should expand D in terms of $\delta = k_{F\uparrow} - k_{F\downarrow}$. The sums are proportional to δ^2 and M is proportional only to δ , so that $D \sim M$. Therefore the spin wave stiffness D is predicted to decrease with the gap Δ and to become zero at the phase transition. Consider, moreover, the complete excitation spectrum. When the spin wave energy becomes equal to the energy of a Stoner excitation, the spin wave can decay into a single particle excitation and is therefore highly damped. Stoner theory therefore predicts that as the gap Δ decreases, the spin waves disappear at lower and lower $|\vec{q}|$ until at the phase transition no spin waves can be seen. We shall soon see that this important prediction is incorrect; its failure provides our strongest impetus for improving the Stoner model.



VI Dynamical Susceptibility

The susceptibility $\chi_{\alpha\beta}(q, \omega)$ tells us the response of the magnetization to an applied space and time dependent magnetic field:

$$\chi_{\alpha\beta}(q, \omega) = \frac{dM_{\alpha}(q, \omega)}{dH_{\beta}(q, \omega)}$$

We can write χ in terms of a retarded Green's function

$$\chi_{\alpha\beta}(q, \omega) = \lim_{\epsilon \rightarrow 0} \int e^{-i(\omega - i\epsilon)(t-t')} \langle\langle S_{\alpha}(q, t), S_{\beta}(-q, t') \rangle\rangle dt(t-t')$$

$\langle\langle S_{\alpha}(q, t), S_{\beta}(q, t') \rangle\rangle$ is the retarded commutator $-i\theta(t-t')\langle[S(q, t), S(-q, t')]\rangle$.

The poles of the transverse susceptibility $\chi_{\alpha\beta}(q, \omega)$ occur at frequencies corresponding to the spin flip normal modes of the system; hence, the susceptibility at small (q, ω) provides another method of finding the spin wave dispersion relation. Moreover, the susceptibility is in itself of interest, because its imaginary part determines the neutron scattering cross section.

If we decompose χ into

$$\begin{aligned} \chi_{+-}(q, t-t') &= \sum_{\mathbf{k}} \langle\langle a_{\uparrow}^{\dagger}(\mathbf{k}) a_{\downarrow}(\mathbf{k}+\mathbf{q})(t); S_{-}(q, t') \rangle\rangle^R \\ &\equiv \sum_{\mathbf{k}} Y(\mathbf{k}, q, t-t') \end{aligned}$$

we can use the following equation of motion:

$$Y(\mathbf{k}, \omega) = \langle[a_{\uparrow}^{\dagger}(\mathbf{k}) a_{\downarrow}(\mathbf{k}+\mathbf{q}), S_{-}(q)]\rangle_{\text{equal times}} + \langle\langle[a_{\uparrow}^{\dagger}(\mathbf{k}) a_{\downarrow}(\mathbf{k}+\mathbf{q}), H], S_{-}(q)\rangle\rangle^R$$

The commutator can be evaluated with H as the usual Hubbard Hamiltonian

$$\text{to give } \{\omega - \epsilon(\mathbf{k}+\mathbf{q}) + \epsilon(\mathbf{k})\}Y(\mathbf{k}) = f_{\uparrow}(\mathbf{k}) - f_{\downarrow}(\mathbf{k}+\mathbf{q})$$

$$\begin{aligned} &- \sum_{\mathbf{k}', \mathbf{k}'' \lambda} \delta(\mathbf{k}, \mathbf{k}') \langle\langle a_{\uparrow}^{\dagger}(\mathbf{k}'+\mathbf{q}) a_{\downarrow}^{\dagger}(\mathbf{k}''-\lambda) a_{\downarrow}(\mathbf{k}'') a_{\downarrow}(\mathbf{k}+\mathbf{q}); S_{-}(-q) \rangle\rangle \\ &- \sum_{\mathbf{k}', \mathbf{k}'' \lambda} \delta(\mathbf{k}+\mathbf{q}, \mathbf{k}''-\lambda) a_{\uparrow}^{\dagger}(\mathbf{k}) a_{\uparrow}^{\dagger}(\mathbf{k}'+\lambda) a_{\uparrow}(\mathbf{k}') a_{\downarrow}(\mathbf{k}''); S_{-}(-q) \rangle\rangle \end{aligned}$$

If the two-particle operator that results from taking the commutator with the two-particle interaction of H is treated in Hartree-Fock, the last two terms will also be susceptibilities; and we find an equation of motion:

$$\begin{aligned} \{\omega - \varepsilon(k+q) + \varepsilon(k) - \Delta\} Y(k) &= f_{\uparrow}(k) - f_{\downarrow}(k+q) \\ &- \{f_{\uparrow}(k) - f_{\downarrow}(k+q)\} U \sum_{k'} Y(k') \end{aligned}$$

We reconstruct χ by summing on \vec{k} :

$$\chi(q, \omega) = \sum_{\vec{k}} \frac{f_{\uparrow}(k) - f_{\downarrow}(k+q)}{\omega - \varepsilon(k+q) + \varepsilon(k) - \Delta} (1 - U\chi) \equiv \chi_0 (1 - U\chi)$$

or
$$\chi(q, \omega) = \chi_0(q, \omega) / (1 + U\chi_0(q, \omega))$$

This result is equivalent to the random phase approximation. If we set the denominator at zero and make (q, ω) small, we shall recognize in the real part of the equation the usual equation for the spin wave.

Now the imaginary part of χ_0 is $-\pi \sum_{\vec{k}} \{f_{\uparrow}(k) - f_{\downarrow}(k+q)\} \delta(\omega - \varepsilon(k+q) + \varepsilon(k) - \Delta)$

and this is non-zero only at the Stoner excitations, which have high energy near $|\vec{q}| = 0$. Hence the spin wave in RPA has infinite lifetime. But at larger $|\vec{q}|$, ω can overlap the Stoner excitations, and the non-zero imaginary part gives the strong damping mentioned above.

We are also interested in the imaginary part of χ ,

$$\text{Im } \chi = \frac{\text{Im } \chi_0}{(1 + U \text{Re } \chi_0)^2 + (U \text{Im } \chi_0)^2}$$

Since $\text{Im } \chi_0 = 0$ at the small (q, ω) for which we wish to evaluate χ , this is equivalent to a standard way of writing the delta function

$$\delta(x) = \lim_{a \rightarrow 0} \frac{a}{x^2 + a^2}$$

Hence

$$\text{Im } \chi = -\pi (n_{\uparrow} - n_{\downarrow}) \delta(\omega - Dq^2) \quad \text{near } |\vec{q}| = 0.$$

VII Experimental Conflicts with Stoner Theory

The Stoner model can describe most of the low temperature behavior of nickel, but there are also some very serious discrepancies with experiment.

(1) Stoner theory does not predict the thermodynamic quantities properly at high temperature. The Stoner theory predicts that above T_C a ferromagnet becomes an ordinary Pauli paramagnet with an enhanced susceptibility; the energy gap, the magnetization, and the magnetic energy become zero together at the transition temperature. The magnetic moments cannot contribute to the entropy above the transition temperature. In a localized model, on the other hand, magnetization fluctuations are present in the macroscopically disordered state; and there is some entropy associated with these degrees of freedom. A great deal of work has recently been done to calculate the critical exponents and amplitudes for Heisenberg models with various values of the spin.^[3] If one attempts to fit the specific heat of nickel to an electronic specific heat calculated from a band structure, one finds that there is a high temperature tail in the entropy above T_C that is not explained by the itinerant model. The specific heat fits very well, however, with Heisenberg model calculations.

(2) The energy gap between the up and down bands does not decrease simply as the average magnetization as it would do in the Stoner theory. Lonzarich and Gold^[4] have used the de Haas-van Alphen effect to look directly at the low temperature shift in the minority spin Fermi level in iron. They found that the change in the gap is very much smaller than one might expect from the change in magnetization at the same

temperature. Now Edwards^[5] has used a Fermi liquid argument to show that the gap ought to change only as $T^{5/2}$ instead of as $T^{3/2}$ in proportion to the magnetization; this result is correct, but it is obtained by guessing the Fermi liquid coefficients and the appropriate spin states of the problem are never defined. Moreover, the Fermi liquid theory is good only for low temperature, and the behavior of the gap must also be understood at high temperature.

(3) At T_C , the band splitting does not become zero as the Stoner theory predicts. This is known from the neutron scattering experiments of Mook, Lynn, and Nicklow.^[6] They found that in nickel spin waves of wave number greater than about 0.2 \AA^{-1} could be seen well above the Curie temperature. If the energy gap were zero at T_C , the spin wave energies at T_C would be in the Stoner continuum for all $|\vec{q}|$ and the spin waves would decay immediately into the Stoner excitations. The maximum spin wave energy is to be identified with the point at which the spin wave dispersion relation first intersects the Stoner continuum. It is constant with temperature above T_C ; if, however, the spin splitting continued to decrease with temperature above T_C , so should the energy at the intersection point. The spin wave stiffness, like the gap, changes only very slowly with temperature, until at T_C it has decreased to half its zero temperature value; above T_C the stiffness is temperature independent over a large temperature range.

VIII Recent Attempts to Account for Magnetization Fluctuations

The Stoner theory provides a self-consistent method of calculating magnetic properties only so long as the single particle Stoner excitations are the most important spin-flip excitations present in the system. In a naive Stoner model, the spin waves are added to the excitation spectrum by hand and are not allowed to interact with each other or with the electrons to change the single particle energies. In fact, the spin wave $T^{3/2}$ term is the most important term of the magnetization, and an acceptable itinerant model must incorporate the spin waves. In principle we could devise a Stoner theory which includes spin waves if we allowed electrons and spin waves to interact to all orders of perturbation theory. Such a calculation would give a Fermi liquid theory with energies:

$$\begin{aligned}\epsilon(k, \sigma) &= \epsilon_0(k, \sigma) + \sum_q f_{em}(k\sigma, q) v(q) + \sum_{k', \sigma'} f_{ee}(k\sigma, k'\sigma') n(k'\sigma') \\ \hbar\omega(q) &= \hbar\omega_0(q) + \sum_{k\sigma} f_{em}(k\sigma, q) \delta n(k\sigma) + \sum_{q'} f_{mm}(q, q') v(q')\end{aligned}$$

However, the renormalizations cannot be done properly. The simplest approximations give up rotational invariance which should be maintained (we know that a $|\vec{q}| = 0$ spin wave is a rotation of the system and cannot change single particle energies) and give unphysically large shifts in the single particle energies.^[7] The general form of the interaction is known (for example, $f_{em}(k\sigma, q) \sim A q^2$). Though the coefficient A is not known, we can make a reasonable guess for the coefficients at low temperature and make a phenomenological Fermi liquid theory. Edwards' calculation of the band splitting mentioned above is a calculation of this sort.^[8]

At high temperatures even such a Fermi liquid theory will not be of use, because the excitations can no longer be described by a simple collection of spin waves.

Near T_C we must deal with local magnetic order and the magnetic degrees of freedom which give rise to the Heisenberg-like magnetic entropy. That there is a considerable energy gap left at T_C indicates that the electrons do interact with the locally ordered magnetization. A method that has been proposed to deal with local order is to make a Stratonovich transformation of variables on the free energy functional integral.^[9] In the new variables single particle energies contain an interaction with a random molecular field. Any Stratonovich transformation has a serious problem however: though formally exact, the functional integral can only be carried out with drastic approximations. There are many forms of the transformation available and the various forms, when approximated, give very different results.

IX Generalization of Stoner Theory

We claim that for itinerant ferromagnets there are really two transitions to be considered. (1) At T_C , the softening of the long wavelength magnetization fluctuations causes the macroscopic magnetization to disappear but allows short range order to persist. (2) Only at a much higher temperature have the single particle Stoner excitations destroyed the population difference between the majority and minority spin bands and with it the energy gap. Then even the short range order disappears and we have a Stoner enhanced paramagnet.

That a short range order of the magnetization persists above the Curie temperature we know, because the spin wave persists above the Curie temperature. The low $|\vec{q}|$ cut-off in the observed spin wave spectrum tells us empirically the size of the region over which short range order must extend. The smallest region a spin wave can see is the size of its wavelength, and it must see an ordered region of magnetization in order to propagate undamped. Hence,

$$q_{\text{short range order}}^{\text{min}} \lesssim q_{\text{spin wave}}^{\text{min}}$$

Now an electron can adjust very quickly to its local environment, so we claim that even in the absence of a macroscopic magnetization, electronic properties are best calculated in a static ordered region. If we do this, the band structure will be characterized by a local order. There will persist a band gap between minority and majority spin bands, but the quantization direction of the spins in these bands will be constant only over regions which sustain a short range order. The majority and minority spin bands will consist of states with spin everywhere essentially parallel and anti-parallel to the local magnetization direction. The phase transition consists in a long range disordering of the magnetization, even while the short range order persists. This is the same as the mechanism for the phase transition in the Heisenberg model, but the electrons themselves are not localized as in the Heisenberg model.

To carry out this idea of how to treat electrons in the presence of short range order, we break the fluctuation spectrum into two parts, the long wavelength fluctuations which contribute to the phase transition and short wavelength fluctuations which

when averaged leave a short range order. This is an idea common in renormalization group theory, to break up the partition function trace:

$$\text{Tr } e^{-\beta H} = \text{Tr}_{q < Q} \text{Tr}_{q > Q} e^{-\beta H}$$

We claim, however, that the physics of the two regions is very different and the two averages must be handled in different approximation schemes. The first trace over the short wavelength fluctuations leaves a free energy $F(\vec{M}(\vec{r}))$ which is a functional of the magnetization configuration. $\vec{M}(\vec{r})$ contains only Fourier components which have not yet been averaged and so varies slowly in space and time. We neglect fluctuations in the magnitude of the magnetization vector as much harder to produce than fluctuations in its direction. Now, before doing the rest of the thermodynamic average, we calculate the single particle and spin wave properties in the presence of this slowly varying magnetization configuration. By the mathematical device of choosing the spin quantization direction to be the direction of the local magnetization, we make the problem essentially the same as the Stoner problem at low temperature. We shall see that, in form, our results look very much like the Stoner model results, with the average macroscopic magnetization $\langle M \rangle$ replaced by the magnitude of the local magnetization $|\vec{M}|$. For example, the gap will not disappear when $\langle M \rangle$ disappears, but will be proportional to $|\vec{M}|$, a quantity which does not disappear until the short range order does at the Stoner temperature.

CHAPTER 2

SINGLE PARTICLE PROPERTIES

In the first chapter, we claimed that properties sensitive to local order should be calculated in the presence of a magnetization which varies slowly in direction. In this chapter, we carry out such a calculation of the single particle properties. Electron energies and eigenstates are found in perturbation theory, with a perturbation Hamiltonian arising from gradients of the magnetization. The eigenstates and energies are essentially the same as those found by Herring and Kittel^[10] in a calculation of the spin wave stiffness and Bloch wall energy. The approximate eigenspinors are not parallel or anti-parallel to the direction of the average magnetization, but rather are approximately parallel or anti-parallel to the direction of the local magnetization. An energy gap is maintained between spin split bands, even when there is no longer a macroscopic magnetization. For low temperature, we can now perform the thermodynamic average over the long wavelength fluctuations; and we find that the gap energy decreases with temperature from its Stoner zero temperature value more slowly than does the average magnetization. The electron energy shifts at the Fermi surface give rise to a shift in the energy difference $\delta\epsilon_{F-} - \delta\epsilon_{F+}$ proportional to the squares of magnetization gradients. This shift drives a repopulation of the spin up and down bands; the repopulation is very similar to the Stoner change in magnetization driven by the temperature shift in chemical potentials. Finally, taking into account the change in energy gap and the repopulation, we

calculate the total energy and free energy of the electrons in the presence of the fluctuations. The differences between these energies and their values in the non-fluctuating ground state are the energies associated with the magnetization fluctuations; the fluctuation free energy takes the expected form of a sum of spin wave energies.

II Electron Eigenstates and Energies

We begin with the Hubbard Hamiltonian

$$H = \sum_{k\sigma} \epsilon(k) n(k,\sigma) + U \sum_{i=\text{sites}} a_{\alpha}^{\dagger}(i) (\vec{\sigma}_{\alpha\beta} \cdot \hat{M}) a_{\beta}(i) a_{\gamma}^{\dagger}(i) (\vec{\sigma}_{\gamma\delta} \cdot \hat{M}) a_{\delta}(i)$$

$\epsilon(k)$ is the spin independent energy of a Bloch state u_k ; $a_{\sigma}^{\dagger}(i)$ is a creation operator of an electron of spin σ in a Wannier state at site i ; and \hat{M} is the magnetization unit vector. The second term in the Hamiltonian is a sum over sites of a Coulomb interaction U between anti-parallel spins at the same site; it has precisely the same form as that part of the Hamiltonian which in Stoner theory makes possible a ferromagnetic equilibrium state. However, we have expressed it in terms of the spatially varying local magnetization unit vector $\hat{M}(r)$, rather than the \hat{z} unit vector which is commonly used. The most important thing about the calculation we are going to do is that, though this Hamiltonian is somewhat more complicated than in the usual Stoner calculation, the dominant effect of the magnetization fluctuations is included trivially, so that we can in effect do what looks like a zero temperature calculation even at temperatures where magnetization fluctuations are important.

To treat single particle properties, we immediately make the Hartree-Fock approximation and write a Schrodinger equation for single electrons:

$$E \Psi = (-\nabla^2/2 + V(r) - \vec{\sigma} \cdot \hat{M}(\vec{r}) \Delta/2) \Psi$$

where $\Delta = |\vec{M}|/U$; the \hat{z} axis is the direction of the expectation of the macroscopic magnetization; and $(-\nabla^2/2 + V(r)) u_k = \epsilon(k) u_k$. The unit vector \hat{M} is to be specified by spatially varying spherical angles, $\theta(r)$ and $\phi(r)$. Notice that we have set the mass m , \hbar , and the volume V of the system to one.

Because the magnetization varies slowly, we wish to use as the unperturbed states in perturbation theory the eigenstates of a Hamiltonian in which the magnetization has magnitude $|\vec{M}|$ but is constant in space and time. Then $\langle \vec{M} \rangle = |\vec{M}| \hat{e}_z$, and the unperturbed Hamiltonian is the usual Stoner ground state Hamiltonian:

$$H_0 = \begin{pmatrix} -\nabla^2/2 - MU/2 & 0 \\ 0 & -\nabla^2/2 + MU/2 \end{pmatrix}$$

It has unperturbed energies $E_{0\pm}(k) = \epsilon(k) \pm MU/2$ and states $u_k \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $u_k \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. In our present frame of reference, where the spins are quantized in the direction of average magnetization, such a scheme is not feasible, because the perturbation Hamiltonian:

$$\delta H(\vec{r}) = \begin{pmatrix} -(MU/2) \cos\theta(\vec{r}) & MU \sin\theta(\vec{r}) e^{i\phi(\vec{r})} \\ MU \sin\theta(\vec{r}) e^{i\phi(\vec{r})} & (MU/2) \cos\theta(\vec{r}) \end{pmatrix}$$

is not necessarily a small perturbation: the only quantities we

assume to be small are gradients of the magnetization. It is still possible to use the unperturbed Hamiltonian above, but to do so we must redefine the spinors $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ by making a rotation to another frame of reference. Physically we expect the eigenstates to follow the local magnetization; and indeed we find that perturbation theory from the eigenstates described above becomes feasible if we transform to a representation where the spins \downarrow and \uparrow are taken to be not $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ but the eigenvectors of $\vec{\sigma} \cdot \hat{M}$:

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \rightarrow R \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\chi_{\uparrow}\rangle = e^{-ib/2} \begin{pmatrix} \cos(\theta(r)/2) e^{-i\phi(r)/2} \\ \sin(\theta(r)/2) e^{+i\phi(r)/2} \end{pmatrix}$$

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \rightarrow |\chi_{\downarrow}\rangle = e^{+ib/2} \begin{pmatrix} -\sin(\theta(r)/2) e^{-i\phi(r)/2} \\ \cos(\theta(r)/2) e^{+i\phi(r)/2} \end{pmatrix}$$

The phase b is the third Euler angle specifying the magnetization and is completely arbitrary. For self-consistency, we require that the expectation of the magnetization in the new occupied states reproduce the assumed magnetization configuration: this constraint will be discussed fully in the next section.

The Hamiltonian in the rotated frame of reference now contains the spatial variation of the magnetization only through the effect of the kinetic energy operator on the spatially varying spinors:

$$RHR^{-1} = \begin{pmatrix} -\nabla^2/2 - MU/2 & \langle \chi_{\downarrow} | -\nabla^2/2 | \chi_{\uparrow} \rangle \\ + \langle \chi_{\uparrow} | -\nabla^2/2 | \chi_{\uparrow} \rangle & + 2 \langle \chi_{\downarrow} | -i\nabla/2 | \chi_{\uparrow} \rangle \cdot (-i\nabla) \\ + 2 \langle \chi_{\uparrow} | -i\nabla/2 | \chi_{\uparrow} \rangle \cdot (-i\nabla) & \\ \\ \langle \chi_{\uparrow} | -\nabla^2/2 | \chi_{\downarrow} \rangle & -\nabla^2/2 + MU/2 \\ + 2 \langle \chi_{\uparrow} | -i\nabla/2 | \chi_{\downarrow} \rangle \cdot (-i\nabla) & + \langle \chi_{\downarrow} | -\nabla^2/2 | \chi_{\downarrow} \rangle \\ & + 2 \langle \chi_{\downarrow} | -i\nabla/2 | \chi_{\downarrow} \rangle \cdot (-i\nabla) \end{pmatrix}$$

The physical interpretation of the rotated Hamiltonian is that the electron still responds to the local magnetization by entering states which follow approximately parallel or anti-parallel to the local magnetization direction; the spatial variation in this direction now requires that some price be paid in kinetic energy for the spatial variation in the spin orientation.

The matrix elements of interest are:

$$\begin{aligned}\langle \chi_{\downarrow} | -i\vec{\nabla} | \chi_{\downarrow} \rangle &= \langle \chi_{\downarrow} | -i\vec{\nabla} | \chi_{\downarrow} \rangle^* = ie^{ib} (\vec{\nabla}\theta/2 - i \sin\theta/2 \vec{\nabla}\phi/2) \\ \langle \chi_{\uparrow} | -\nabla^2 | \chi_{\uparrow} \rangle &= | -i\vec{\nabla} \chi_{\uparrow} |^2 = \{ (\nabla\theta/2)^2 + (\nabla\phi/2)^2 + (\nabla b/2)^2 - 2\cos\theta \vec{\nabla}\phi/2 \cdot \vec{\nabla}b/2 \} \\ \langle \chi_{\downarrow} | -\nabla^2 | \chi_{\downarrow} \rangle &= | -i\vec{\nabla} \chi_{\downarrow} |^2 = \{ (\nabla\theta/2)^2 + (\nabla\phi/2)^2 + (\nabla b/2)^2 + 2\cos\theta \vec{\nabla}\phi/2 \cdot \vec{\nabla}b/2 \}\end{aligned}$$

In its most convenient form the perturbing Hamiltonian is written:

$$\begin{pmatrix} a^2/2 + (-i\vec{\nabla} + \vec{A})^2/2 + \nabla^2/2 & -ie^{+ib} \vec{a} \cdot (-i\vec{\nabla}) \\ ie^{-ib} \vec{a}^* \cdot (-i\vec{\nabla}) & a^2/2 + (-i\vec{\nabla} - \vec{A})^2 + \nabla^2/2 \end{pmatrix}$$

We have defined $\vec{a} \equiv \vec{\nabla}\theta/2 + i \sin\theta \vec{\nabla}\phi/2$

and $\vec{A} = (\vec{\nabla}b + \cos\theta \vec{\nabla}\phi)$

We can now make use of the arbitrariness of the phase b to simplify

the Hamiltonian further: we require that \vec{A} be transverse, that is,

$$\vec{\nabla} \cdot \vec{A} = 0. \quad \text{Hence} \quad \vec{\nabla} \cdot \vec{A} = \nabla^2 b + \vec{\nabla} \cdot \cos\theta \vec{\nabla}\phi = 0$$

or b is chosen as $\int \frac{d^3 r'}{4\pi |\mathbf{r}-\mathbf{r}'|} (\vec{\nabla}_{\mathbf{r}'} \cdot \cos(\theta(\mathbf{r}')) \vec{\nabla}_{\mathbf{r}',\phi}(\mathbf{r}'))$

$$= \vec{\nabla}_{\mathbf{r}} \cdot \int \frac{d^3 r'}{4\pi |\mathbf{r}-\mathbf{r}'|} \cos\theta \vec{\nabla}\phi \equiv \vec{\nabla} \cdot \vec{\mathcal{I}} \quad .$$

Then $\vec{\nabla}b = \vec{\nabla}(\vec{\nabla} \cdot \vec{\mathcal{I}}) = \vec{\nabla} \times \vec{\nabla} \times \vec{\mathcal{I}} - \nabla^2 \vec{\mathcal{I}}$

and we find $\vec{A}(\mathbf{r}) = \int \frac{d^3 r'}{4\pi |\mathbf{r}-\mathbf{r}'|} \vec{\nabla}_{\mathbf{r}'} \times (\vec{\nabla}_{\mathbf{r}'} \cos\theta \times \vec{\nabla}_{\mathbf{r}',\phi})$

Though the $\vec{A}(\mathbf{r})$ terms of the Hamiltonian give rise to real scattering of electrons, they can be ignored in the present calculation of the change in band structure and energy gap. Two things are required if \vec{A} is to be ignored: though \vec{A} may alter the motion of the individual electrons, it must not alter the underlying band structure and must be able to be treated independently of the band structure; and its contribution to the total electronic energy must be zero at least to second order in the magnetization gradients.

To demonstrate that the first statement is true, we notice that \vec{A} enters the Hamiltonian as an effective magnetic vector potential, and we apply to it the usual treatment of the effect of weak magnetic fields on conduction electrons. The magnetic field is to be taken account of in the effective mass approximation, as in the standard calculations of the Landau diamagnetic susceptibility or cyclotron resonance. The basic idea is to find an approximate Bloch state of wavevector \vec{k} from the solution at $\vec{k} = 0$. One derives an effective Hamiltonian

$$H = \left(\vec{k} - \frac{e\vec{A}}{c} \right) \cdot \frac{m^{-1}}{2} \cdot \left(\vec{k} - \frac{e\vec{A}}{c} \right) + V(\mathbf{r})$$

where $\vec{A}(\mathbf{r})$ and $V(\mathbf{r})$ are slowly varying applied potentials, and $V(\mathbf{r})$ is zero for our case. The only requirement for the derivation of such a Hamiltonian is that the vector potential $\vec{A}(\mathbf{r})$ be slowly varying over the space of a unit cell, a requirement certainly met by $\vec{A}(\mathbf{r})$. The effect of the periodic lattice potential is all contained in the inverse mass tensor m^{-1} ; m^{-1} is, moreover, purely a band property and independent of the external fields. Now it can be shown that the crystal momentum \vec{k} can be treated as it if were the actual classical

momentum of an electron. A conduction electron behaves like a wave packet of momentum \vec{k} and group velocity $\vec{v} = \vec{v}_k$ which obeys the equation of motion $\dot{\vec{k}} = e \vec{v} \times \vec{H}$; and it traces out orbits on surfaces of constant energy in k-space. The result that we want to use is that in the presence of slowly varying fields, the band structure of the conduction electrons is calculated first in the absence of such fields, and then the response to the fields can be treated without modifying the band calculations. In particular, $\vec{A}(r)$ does induce transitions between states but this has no effect on the Bloch states and band energy changes we wish to calculate.

If now we find the effect of \vec{A} on the total electronic energy by doing second order perturbation theory, we find that in the total energy the first and second order contributions, each of order A^2 , cancel each other. This effect is again most easily understood in terms of equivalent magnetic fields. The contribution of a magnetic field to the total energy is the same energy that enters the calculation of the Landau diamagnetic susceptibility, and it is of order H^2 . $(\vec{v} \times \vec{A})^2$ is fourth order in magnetization gradients and can be ignored.

Therefore we consider only the perturbation Hamiltonian:

$$\begin{pmatrix} \frac{1}{2} a^2 & -e^{ib} i\vec{a} \cdot (-i\vec{v}) \\ e^{-ib} i\vec{a}^* \cdot (-i\vec{v}) & \frac{1}{2} a^2 \end{pmatrix}$$

the diagonal term in first order and the terms proportional to $\sigma_{+,-}$ in second order. The Bloch state $\psi_{k\uparrow}(r) = u_k(r)\chi_{\uparrow}(r)$ becomes

$$\psi_{k\uparrow}(r) \rightarrow \psi_{k\uparrow}(r) + \sum_{k'} \int d^3r \frac{\langle u_{k'}(r) | -i\vec{a} \cdot (-i\vec{v}) e^{ib} | u_k(r) \rangle}{\epsilon_{\uparrow}(k') - \epsilon_{\downarrow}(k)} \langle \chi_{\uparrow}(r) | \frac{1}{2} \sigma_{+} | \chi_{\downarrow}(r) \rangle$$

The momentum change ($\vec{k}' - \vec{k}$) caused by the factor e^{ib} is again a magnetization gradient. Since the matrix element already goes as \vec{a} , also a magnetization gradient, we can consider the transition to be vertical and drop the factor e^{ib} . Then, using

$$\int d^3r u_k(r) (-i\vec{\nabla}) u_k(r) = \vec{v}_k$$

we find the new normalized eigenstates to be

$$\begin{aligned}\psi_+(k) &= \psi_{\uparrow}(k) \cos \frac{\vec{v}_k \cdot \vec{a}}{\Delta} - \psi_{\downarrow}(k) \sin \frac{\vec{v}_k \cdot \vec{a}}{\Delta} \\ \psi_-(k) &= \psi_{\downarrow}(k) \cos \frac{\vec{v}_k \cdot \vec{a}}{\Delta} + \psi_{\uparrow}(k) \sin \frac{\vec{v}_k \cdot \vec{a}}{\Delta}\end{aligned}$$

Similarly the perturbed energies are:

$$E_{\pm}(k) = \epsilon(k) \mp \frac{1}{2} \langle M \rangle U \mp (\vec{v}_k \cdot \vec{a}) / \Delta + \frac{1}{2} a^2$$

The eigenstates almost follow the local magnetization direction, but are slightly tilted away from it. Our expansion parameter is $\vec{v} \cdot \vec{a} / \Delta$. The condition that it be small, $v_F a / \Delta \ll 1$, means that the range of the short range order must be greater than about 30 Å for nickel. This defines the separation between the long and short wavelength fluctuations.

III Change in Energy Gap and Repopulation of the Bands

The magnitude of the magnetization vector $\langle n_{\uparrow} - n_{\downarrow} \rangle$ is now no longer equal to the population difference between the spin split bands, but can be calculated in a state $|\phi'\rangle$ given by populations of the eigenstates ψ_+ and ψ_- .

$$\begin{aligned}
n_{\uparrow} - n_{\downarrow} &= \langle \Phi' | \sum_{\mathbf{k}} (n_{\uparrow}(\mathbf{k}) - n_{\downarrow}(\mathbf{k})) | \Phi' \rangle \\
&= \sum_{\text{all}} |\langle \psi_{\mathbf{k}\sigma} | \psi_{\mathbf{k}\uparrow} \rangle|^2 - |\langle \psi_{\mathbf{k}\sigma} | \psi_{\mathbf{k}\downarrow} \rangle|^2 \\
&= \sum_{\text{so}} \cos^2 \left(\frac{\vec{\mathbf{a}} \cdot \vec{\mathbf{v}}(\mathbf{k})}{\Delta} \right) - \sin^2 \left(\frac{\vec{\mathbf{a}} \cdot \vec{\mathbf{v}}(\mathbf{k})}{\Delta} \right) \\
&= n_{+} - n_{-} - 2 \sum_{\text{so}} (\vec{\mathbf{a}} \cdot \vec{\mathbf{v}}(\mathbf{k}))^2 / \Delta
\end{aligned}$$

We must next determine the population $n_{+}-n_{-}$ in terms of a population difference $n_{\uparrow}^0 - n_{\downarrow}^0$ of a non-fluctuating, or zero temperature, ground state. If we consider the magnetization fluctuations to be turned on adiabatically, Rayleigh-Schrodinger perturbation theory tells us that the unperturbed eigenstates $\psi_{\uparrow}(\mathbf{k})$ and $\psi_{\downarrow}(\mathbf{k})$ will pass adiabatically into the eigenstates $\psi_{+}(\mathbf{k})$ and $\psi_{-}(\mathbf{k})$. These populations, however, do not correspond to thermodynamic equilibrium. For, consider the part of the perturbed energy $(\vec{\mathbf{v}} \cdot \vec{\mathbf{a}})^2 / \Delta$: This piece of the energy in effect reduces the effective mass of the (-) spin band, and at fixed n_{-} lowers the chemical potential. Since $|\vec{\mathbf{v}}(\mathbf{k})|$ is different at the + spin Fermi wavevector, the shift in chemical potential at fixed occupation of the (+) spin band is different from that of the (-) spin band. Therefore there must take place some repopulation of the two bands to keep $\delta\mu_{+} = \delta\mu_{-}$. The calculation of the repopulation must self-consistently take into account the change in $\Delta = \langle |M| \rangle U$ as well, just as in the Stoner calculation of the change in magnetization with temperature.

There are three contributions to the shift in chemical potential $\delta\mu_{+}$: the explicit change from the repopulation $\delta n_{+} / N_{+}$, the change

in chemical potential at constant number arising from the perturbed energy which is $-\oint_{\epsilon_+} |v| d\Omega (\vec{a} \cdot \vec{v})^2 / \Delta N_+$, and the change in energy

evaluated at the Fermi surface arising from the change in magnetization magnitude, $-\frac{1}{2}(\delta n_+ - \delta n_-)U - U \int_{so} (\vec{a} \cdot \vec{v})^2 / \Delta^2$. Thus

$$\begin{aligned} \delta \mu_+ &= -\frac{1}{2} \delta(n_+ - n_-)U - \oint_{\epsilon_+} \frac{da}{|v|} (\vec{a} \cdot \vec{v})^2 / \Delta N_+ + \delta n_+ / N_+ + U \int_{so} (\vec{a} \cdot \vec{v})^2 / \Delta^2 \\ &= \delta \mu_- = +\frac{1}{2} \delta(n_+ - n_-)U + \oint_{\epsilon_-} \frac{da}{|v|} (\vec{a} \cdot \vec{v})^2 / N_- + \delta n_- / N_- - U \int_{so} (\vec{a} \cdot \vec{v})^2 / \Delta^2 \end{aligned}$$

δn_+ must equal $-\delta n_-$ if the total number of electrons is to be unchanged, and so we find that

$$\delta(n_+ - n_-) = 2 \frac{\frac{1}{N_+} \oint_{\epsilon_+} |v| d\Omega \frac{(\vec{v} \cdot \vec{a})^2}{\Delta} + \frac{1}{N_-} \oint_{\epsilon_-} |v| d\Omega \frac{(\vec{v} \cdot \vec{a})^2}{\Delta} - \frac{2}{M} \int_{so} d\epsilon \oint_{\epsilon} |v| d\Omega \frac{(\vec{v} \cdot \vec{a})^2}{\Delta}}{\frac{1}{N_+} + \frac{1}{N_-} - 2U}$$

In the strong limit, however, there is an energy gap $\Delta - \mu$ between the bottom of the empty (-) spin band and the uppermost occupied level in the (+) spin band. Hence the shift in chemical potential is simply the shift in μ_+ at constant n_+ , and there is no repopulation in the strong limit. We can also see this from the expression above, since in the strong limit $N_- = 0$, giving an infinite denominator.

The energy gap is defined to be the energy necessary to flip a spin from (-) to (+) without changing its momentum. The shift in gap from its value in the absence of magnetization fluctuations is \vec{k} -dependent:

$$\delta\Delta(k) = \delta(n_+ - n_-)U + 2(v_k \cdot a)^2/\Delta - 2 \sum_{so} (v_k \cdot a)^2/M\Delta$$

The first term comes explicitly from the repopulation and the rest from the perturbed energy and change in magnetization magnitude. The change in gap is not only small because it is proportional to the square of the magnetization gradients; when it is averaged over the singly occupied states it is equal to $\delta(n_+ - n_-)U$ only, and its average is strictly zero in the strong limit.

IV Thermodynamics

We have so far found the shift in gap and magnetization $|\vec{M}|$ in terms of the magnetization gradients $|\vec{a}|^2 = \frac{1}{4}|\vec{V}\theta + i \sin\theta \vec{V}\phi|^2$. If we want to find the temperature dependence of these quantities to compare them to the Stoner results and experiment, we must perform the thermodynamic average over the fluctuations.

At low temperature and small angle θ , when there are not many spin waves present in the system and the spin waves do not interact, the average can easily be done in terms of single spin waves. If a single spin wave of wavevector \vec{q} is present in the system, $\vec{q} = \vec{V}\phi$ and $|\vec{a}| = |\vec{V} \sin\theta e^{i\phi}| = |\vec{V}M^+|$. The angle θ is given in terms of the number of such spin waves present by

$$\cos\theta = \frac{M_0 - 2v(q)}{M_0}$$

where $v(\vec{q})$ is the number of spin waves of \vec{q} at temperature T . Hence

$$\sin\theta = 4v(q)/M_0$$

The average is taken by summing over the spin waves with $v(q)$ equal to

the usual Bose factor $(\exp \frac{Dq^2}{kT} - 1)^{-1}$.

For simplicity we shall not include the repopulation terms, which have the same temperature dependence as the rest. Then at low temperature, the spin wave sums can be taken to infinity and

$$\begin{aligned}\delta \langle M \rangle &= 2 \sum_q v(q) \\ \delta |M| &= - \frac{2v(q)}{M} \sum_{so} \frac{(\vec{v} \cdot \vec{q})^2}{\Delta} = - \frac{2}{3} \{ \overline{v^2} / \Delta \} \sum_q v(q) q^2 \\ \delta \Delta_v &= 2 \sum_q v(q) \left(\frac{(\vec{v} \cdot \vec{q})^2}{\Delta} - \frac{2}{M} \sum_{so} \frac{(\vec{v} \cdot \vec{q})^2}{\Delta} \right) .\end{aligned}$$

The average magnetization is proportional to $T^{3/2}$ whereas the gap and magnetization magnitude decrease only as $T^{5/2}$.

It is now interesting to compare these results to Edwards' [5] Fermi liquid theory estimate for the temperature dependence of the de Haas-van Alphen frequency. The gap shift of interest to Edwards is not the gap for vertical transitions which we have calculated, but the quasi-particle energy $\epsilon_{F-} - \epsilon_{F+}$, or an average gap shift defined as $\frac{1}{2N_+} \oint_{\epsilon_+} |v| d\Omega \delta\Delta(k) + \frac{1}{2N_-} \oint_{\epsilon_-} |v| d\Omega \delta\Delta(k)$

Edwards calculates this in the weak limit and finds

$$\begin{aligned}\delta \Delta_E &= 2 \frac{D}{M} \sum_q v(q) q^2 \\ &= \frac{2}{M} \sum_q v(q) \left(\oint_{\epsilon_+} |v| d\Omega \frac{(\vec{v} \cdot \vec{q})^2}{\Delta} + \oint_{\epsilon_-} |v| d\Omega \frac{(\vec{v} \cdot \vec{q})^2}{\Delta} \right. \\ &\quad \left. - \frac{2}{\Delta} \int_{so} d\epsilon \oint |v| d\Omega \frac{(\vec{v} \cdot \vec{q})^2}{\Delta} \right)\end{aligned}$$

Our result for this quasi-particle energy is

$$\frac{1}{M} \sum_q v(q) \left(\left\{ \frac{1}{N_+} \phi_{\epsilon_+} + \frac{1}{N_-} \phi_{\epsilon_-} - \frac{2}{M} \int_{so} d\epsilon \phi_{\epsilon} \right\} (v \cdot q)^2 / \Delta \right)$$

Evaluated in parabolic bands, this is 3/2 of Edwards' result.

As opposed to Edwards, we have calculated the change in the population difference $n_+ - n_-$ self-consistently, with the energy difference above as the driving force. This brings in the enhancement factor

$$(1/N_+ + 1/N_- - 2U)^{-1}$$

which changes the coefficient of the temperature quite a bit. In fact, it is this factor which causes the repopulation to vanish in the strong limit. The temperature dependence of the quasi-particle energy, however, is $T^{5/2}$ for both calculations.

In summary, we find that the local properties of the electrons, the band splitting and local magnetization, are relatively insensitive to the long range disorder that changes the expectation of the magnetization, decreasing much more slowly with temperature. The relevant quantity in the calculations is not $\langle M \rangle$, but rather the occupation of the spin eigenstates $n_+ - n_-$, which decreases with temperature only through the direct repopulation of the bands, either through the Stoner T^2 mechanism or the repopulation effect discussed above. In the strong limit, both effects are negligible until high temperatures.

At high temperatures many spin waves are present in the system, and the averages of the magnetization gradients must be replaced by

functional averages, done with the constraint that the magnitude of the magnetization does not fluctuate. We have not carried out these functional averages, because the constraint represents a mathematical problem of great difficulty. The low temperature behavior indicates that local properties are relatively insensitive to the temperature and this qualitative result can be expected to hold through the Curie point.

V Spin Wave Stiffness and Fluctuation Free Energy

The difference between the total energy in the presence of the fluctuating background and the energy in the non-fluctuating ground state is the energy of the fluctuations themselves; and similarly for the free energy. The free energy is of interest for two reasons. First, it is needed for the thermodynamic average over magnetization configurations. As we mentioned in the last section, a function of M , $O(M)$, is averaged with the functional integral,

$$\int \mathcal{D}M e^{-F(M)/kT} O(M)$$

with $F(M)$ the free energy. Second, the free energy determines the Landau-Lifshitz equation of motion for the magnetization. If we find the coefficient of $|\nabla M|^2$ in the free energy

$$\delta F = A |\nabla M|^2 / M^2$$

this determines an effective magnetic field

$$\vec{H}_{\text{eff}} = - \frac{2A}{M^2} \nabla^2 \vec{M}$$

to which the magnetization can be assumed to respond gyroscopically.

This gives an equation of motion

$$\frac{\partial \vec{M}}{\partial t} = - \vec{M} \times \frac{2A}{M} \nabla^2 \vec{M} .$$

We expect this to be the usual Landau-Lifshitz equation

$$\frac{\partial \vec{M}}{\partial t} = - D \vec{M} \times \nabla^2 \vec{M}$$

and hence that the free energy is proportional to the usual RPA spin wave stiffness.

To find the total energy to $O(a^2)$ we must take into account

- (1) terms in the eigenenergies that are explicitly proportional to a^2 ,
- (2) the energy change arising from the repopulation of levels, and
- (3) a change in the kinetic energy $\sum_{k, \sigma=+, -} \epsilon(k) n(k, \sigma)$ arising from

the shift in chemical potential and from the replacement of Fermi factors $f_{\uparrow, \downarrow}(\epsilon(k))$ by $f_{+, -}(E_{+, -}(k))$.

The repopulation makes no contribution to the total energy of order δM : it causes a change in kinetic energy

$$\epsilon_+ \delta n_+ + \epsilon_- \delta n_- = \frac{1}{2} \delta M (\epsilon_+ - \epsilon_-) = \frac{1}{2} \delta M \Delta$$

and a change in magnetic energy $-\frac{1}{4} (2M \delta M) U = -\frac{1}{2} \delta M \Delta$.

Therefore the contribution of the repopulation is only of order $(\delta M)^2$, or order a^4 . We must also include the effect of an arbitrary deviation of M from its Stoner equilibrium value, which is calculated in the same way as the effect of repopulation. Again, therefore, there is no contribution of order δM to the energy. The contribution of order $(\delta M)^2$ can easily be evaluated by considering the deviation of the population difference from its Stoner value to constitute an effective magnetic field, $\delta H = U \delta M / \mu_B$. The contribution of the field

to the energy is $-\frac{1}{2}(\delta M)(\delta H) = \frac{1}{2}(\delta M)^2/\chi$. Precisely as in Section III of Chapter 1, χ is the Stoner enhanced paramagnetic susceptibility.

Next we calculate the contribution from the a^2 terms of the perturbed energies. We cannot simply add the single particle energies

$$E_{\pm}(k) = \epsilon(k) + \frac{1}{2}a^2 \mp |M|U \mp (\vec{a} \cdot \vec{v})^2/\Delta$$

because this would count magnetic interactions twice. Rather, we should use the full Hamiltonian:

$$\begin{aligned} H = & \sum_{\vec{k}, \sigma=\pm} E(k, \sigma) n(k, \sigma) + \frac{1}{2} \sum_{\vec{k}} n_{\uparrow}(\vec{k}) - n_{\downarrow}(\vec{k}) \\ & + U \sum_{\vec{k}, \vec{k}', \vec{q}} a_{\uparrow}^{\dagger}(\vec{k}+\vec{q}) a_{\uparrow}(\vec{k}) a_{\downarrow}^{\dagger}(\vec{k}'-\vec{q}) a_{\downarrow}(\vec{k}') \end{aligned}$$

In this expression for H , the exchange energy is replaced by its Fourier transform representation. Note that the single particle terms are now written in the eigenstate representation, but the exchange energy involves not the eigenspinors but the spinors which are parallel and anti-parallel to the local magnetization. The expectation of this Hamiltonian in a state given by populations of (+) and (-) electrons will give the total energy in the presence of fluctuations.

$$\begin{aligned} \delta E = & \sum_{\text{all}} \frac{1}{2}a^2 + \sum_{\text{so}} (\vec{v} \cdot \vec{a})^2/\Delta - \sum_{\text{so}} (\vec{v} \cdot \vec{a})^2/\Delta \\ & - 2 \sum_{\text{so}} (\vec{v} \cdot \vec{a})^2/\Delta \\ & + \sum_{\text{so}} (\vec{v} \cdot \vec{a})^2/\Delta \\ = & \sum_{\text{all}} \frac{1}{2}a^2 - \sum_{\text{so}} (\vec{v} \cdot \vec{a})^2/\Delta = M D a^2 \end{aligned}$$

D is the standard RPA expression for the spin wave stiffness.

At $T=0$ there is no contribution from the change in kinetic energy described above in (3): the change arising from the shift in chemical potential exactly cancels that arising from the change in Fermi factors. MDa^2 is thus the fluctuation energy, and also the free energy $E - TS$.

At $T > 0$, the chemical potential shift is driven by both the temperature and a^2 , and for low temperature $\delta\mu$ is

$$\delta\mu = -\frac{\pi^2 T^2}{6\mu_0} - \frac{a^2 \mu_0}{3\Delta} - \frac{a^2 \pi^2 T^2}{9\Delta \mu_0}$$

For simplicity, we evaluate $\delta\mu$ and δE in the strong limit. The corresponding change in the kinetic energy is $\frac{4a^2 \pi^2 T^2}{9\Delta \mu_0}$.

The temperature dependence of MDa^2 is $-\frac{2a^2 \pi^2 T^2}{9\Delta \mu_0}$. Hence

$E = MDa^2$ but contains the temperature dependent term with the opposite sign.

It is rather the free energy that contains MDa^2 . The entropy can be evaluated by using the thermodynamic relation, $T \frac{dS}{dT} = \frac{dE}{dT}$.

The temperature dependent part of $F = E - TS$ is $-\frac{2a^2 \pi^2 T^2}{9\Delta \mu_0}$.

The fluctuation free energy can now be written:

$$F = MDa^2 + (M - M_0)^2 / 2\chi.$$

This free energy also has the satisfying property that if we minimize the free energy with respect to the number difference $n_+ - n_-$ we find that the equilibrium number difference is exactly the result of page 28, which we found in an entirely different fashion. That the free energy is to be minimized with respect to the number difference, rather than the average magnetization or local magnetization

magnitude, gives support to the idea that it is the number difference between the spin eigenstates that is the significant parameter of the problem, rather than the average magnetization or magnetization magnitude.

CHAPTER 3

SPIN WAVES IN THE PRESENCE OF MAGNETIZATION FLUCTUATIONS

Armed with our knowledge of the eigenstates and energies in the presence of slow magnetization fluctuations, we can now treat the effect of such fluctuations on the collective spin flip excitation.

In the Stoner ground state, where the magnetization does not vary in space or time, the collective excitation consists of a small differential rotation of the magnetization vector; the magnetization is tilted away from its initial direction by a small angle and rotated about that direction with a phase $\vec{Q} \cdot \vec{r} - \omega(Q)t$. We have seen that even when the magnetization direction varies in space and time, the electrons behave very much as if the magnetization were not fluctuating: the spins tend to align with the local direction of the magnetization and the spin band gap is almost unaltered. We therefore expect a spin flip excitation to rotate the magnetization as it did in the simpler case, but now away from its local direction. In terms of a wave function for the excited state, we expect that the RPA wave function of Chapter 1, page 9, $\sum_p c_p a_{\downarrow}^{\dagger}(p+Q) a_{\uparrow}(p) |\Phi_0\rangle$, can be taken over, at least approximately, if \uparrow and \downarrow are taken to mean up and down with respect to the local magnetization direction.

This wave function could indeed be taken over directly if the spin eigenstates $+$ and $-$ were identical to the locally defined \uparrow and \downarrow states and the eigenenergies were precisely $E_{\mp}(k) = \epsilon(k) \pm \Delta/2$. The Hamiltonian would then have precisely the same form as the Hubbard Hamiltonian of the Stoner ground state and hence give rise to the same

collective excitation.

The wave function cannot be taken over directly because of the presence in the Hamiltonian of the two vector parameters which characterize the background fluctuations, \vec{A} , an effective magnetic vector potential, and \vec{a} , the magnetization gradient $(\vec{\nabla}\theta + i \sin\theta \vec{\nabla}\phi)/2$. Suppose we make an excitation of the form $a_{\alpha}^{\dagger}(p+Q) a_{\beta}(p) |\phi_0\rangle$ in the presence of the fluctuations. We shall find that the vector \vec{a} , the coefficient of the σ_+ and σ_- components of the Hamiltonian, mixes it with excitations of different spin indices and that \vec{A} mixes it with excitations of different momenta \vec{Q}' . These two effects correspond to a scattering of the spin wave with the single particle, spin-conserving excitations and with other spin waves. Because \vec{a} and \vec{A} disturb the excitation differently, the two effects can be treated separately. In this chapter, we shall consider the effect only of the magnetization gradient \vec{a} .

The interaction between the spin wave and the slower magnetic fluctuations of the background give rise to a spin wave lifetime and a change in the spin wave stiffness D . The spin wave dispersion relation is expected to be of the general form

$$\omega(Q) = D_0 Q^2 + B a^2 Q^2 + C(\vec{a} \cdot \vec{Q})^2.$$

The problem to be treated in this chapter is the calculation of the coefficients C and B . If \vec{a} is taken to correspond to a single spin wave, these coefficients provide an expression for the Fermi liquid parameter $b(Q, Q')$ in the Fermi liquid energy:

$$\omega(Q) = \omega_0(Q) + \sum_k \delta n(k) a(k, Q) + \sum_{Q'} v(Q') b(Q', Q) .$$

The problem of calculating the Fermi liquid parameter $b(Q, Q')$ has previously been treated by Izuyama and by Kawasaki^[11]. In their formulations, a state of two spin waves of momenta \vec{p} and \vec{q} is taken to be produced by the product of the usual RPA spin wave creation operators $A^\dagger(p)$ and $A^\dagger(q)$. These operators each satisfy the equation

$$[H, A^\dagger(p)] |\phi_0\rangle = \omega A^\dagger(p) |\phi_0\rangle$$

but not as an operator relation, only when the state ϕ_0 is the ground state. In this scheme, the interaction energy of the two spin waves is a result of the non-commutivity of the spin wave creation operators; and the Fermi liquid coefficient is $\langle \phi_0 | [A(p), [A(q), [H, A^\dagger(q)], A^\dagger(p)]] | \phi_0 \rangle$. This sort of calculation does not include the effect of any perturbation on the wave function of the excitation.

We do an RPA calculation of the collective spin flip excitation of momentum \vec{Q} in a system with a background magnetization fluctuation. We take account of the background by using the eigenstates and energies previously computed, and a Hamiltonian which takes account of the altered dynamics associated with the vector perturbation parameter \vec{a} . We use our knowledge of the eigenstates to write the Hamiltonian in the following form:

$$H = \sum_k \{E_+(k)n_+(k) + E_-(k)n_-(k)\} + U \sum_i n_{i\uparrow}n_{i\downarrow} + \frac{1}{2}U \langle n_\uparrow - n_\downarrow \rangle \sum_k (n_\uparrow(k) - n_\downarrow(k)).$$

The first term is the $(+,-)$ eigenstate representation of the Hartree-Fock single particle energy treated in Chapter 2. The second term reinstates the magnetic interaction $-\sigma_z MU/2$ as the full two-particle interaction; the last term subtracts from the Hubbard interaction its approximation in Hartree-Fock, which is already included in the eigenenergies $E_{+,-}$.

We can find the collective excitation by minimizing the expectation of this Hamiltonian in a trial wave function for the excited state, as on page 9 . We might try to take as the spin flip excitation a variational wave function of the form

$$A^\dagger(Q) |\Phi_0\rangle = \sum_p c_p a_-^\dagger(p+Q) a_+(p) |\Phi_0\rangle$$

In a system where \uparrow and \downarrow are identical with $+$ and $-$, this wave function is an appropriate start for a variational calculation; but this is true only because the Hamiltonian

$$U \sum_{k,k',q} a_\uparrow^\dagger(k+q) a_\uparrow(k) a_\downarrow^\dagger(k'-q) a_\downarrow(k')$$

does not mix the spin flip excitation with the spin conserving excitations $a_+^\dagger(p+Q) a_+(p) |\Phi_0\rangle$ and $a_-^\dagger(p+Q) a_-(p) |\Phi_0\rangle$. Now, however, because \uparrow and \downarrow contain a mixture of spins $+$ and $-$, the Hamiltonian does have matrix elements among these excitations, and a variational state must also include some admixture of these excitations:

$$A^\dagger(Q) |\Phi_0\rangle = \sum_p \left[c_p a_-^\dagger(p+Q) a_+(p) + u_p a_+^\dagger(p+Q) a_+(p) + d_p a_-^\dagger(p+Q) a_-(p) \right] |\Phi_0\rangle$$

The equations of motion for the coefficients c_p , u_p , and d_p are now coupled together.

We can do precisely the same calculation by looking for a pole in the dynamical susceptibility

$$\chi_{+-}(Q, \omega) \equiv \sum_p \langle\langle a_+^\dagger(p+Q) a_-(p); S_-(-Q) \rangle\rangle^R,$$

and this is the form in which the calculations will be presented. The perturbation in the wave function of the spin wave corresponds to coupling between the susceptibilities χ_{+-} and

$$\chi_{\sigma\sigma}(Q, \omega) \equiv \sum_p \langle a_{\sigma}^{\dagger}(p+Q) a_{\sigma}(p); S_{-}(-Q) \rangle^R.$$

We must stipulate that the excitation whose dispersion relation we calculate be of shorter wavelength than the fluctuations of the background. If the background varies faster than the excitation superposed on it, it will be a serious error to ignore the time dependence of the background fluctuations.

Some care also must be taken in including a coupling with the susceptibilities χ_{++} and χ_{--} , or with the wave functions $a_{+}^{\dagger}(p+Q) a_{+}(p)$ and $a_{-}^{\dagger}(p+Q) a_{-}(p)$. The susceptibility $\chi_{\rho} \equiv \chi_{++} + \chi_{--}$ itself actually has a pole at the plasma frequency which does not appear in our calculation because we have used an effective short ranged potential. This is a very high frequency excitation and its contribution to the spin wave dispersion relation is suppressed. Therefore, we must constrain the variational wave function not to contain density oscillations, or the susceptibility not to interact with that part of χ_{++} and χ_{--} which gives rise to the plasmon. The coupling with the density oscillations can and will be removed explicitly from the equations of motion.

II Equations of Motion for the Dynamical Susceptibility

We define a dynamical susceptibility

$$\begin{aligned}\chi_{\alpha\beta}(Q, \omega) &\equiv \sum_p \chi_{\alpha\beta}(p, Q, \omega) \\ &= \sum_p \int d(t-t') e^{i\omega(t-t')} \langle\langle a_{\alpha}^{\dagger}(p+Q) a_{\beta}(p)(t); S_{-}(-Q, t') \rangle\rangle^R\end{aligned}$$

and find the spin wave dispersion relation by finding a pole at low frequency in the susceptibility $\chi_{+-}(Q, \omega)$. The equation of motion for $\chi_{\alpha\beta}(p, Q, \omega)$ is

$$\begin{aligned}\omega \chi_{\alpha\beta}(p, Q, \omega) &= \langle\langle a_{\alpha}^{\dagger}(p+Q) a_{\beta}(p); S_{-}(-Q) \rangle\rangle_{\text{equal times}} \\ &\quad + \langle\langle [a_{\alpha}^{\dagger}(p+Q) a_{\beta}(p), H]; S_{-}(-Q) \rangle\rangle^R.\end{aligned}$$

Because we are looking for a pole in χ_{+-} , we can ignore the equal times commutator as an inhomogeneous term.

The result of taking the commutator $[a_{\alpha}^{\dagger}(p+Q) a_{\beta}(p), H]$ is a two-particle operator; if this is treated in the Hartree-Fock approximation, the commutator can be written again in terms of susceptibilities and we find equations of the general form

$$\begin{aligned}\omega \chi_{\alpha\beta}(p, Q, \omega) &= \{E_{\beta}(p) - E_{\alpha}(p+Q)\} \chi_{\alpha\beta}(p) \\ &\quad - \{f_{\alpha}(p+Q) - f_{\beta}(p)\} \sum_{p'} \Gamma_{\alpha\beta, \mu\nu}(p, p') \chi_{\alpha\beta}(p')\end{aligned}$$

In general $\Gamma_{\alpha\beta, \mu\nu}$ is a function of both \vec{p} and \vec{p}' and is non-zero for all values of the indices $\alpha\beta, \mu\nu$. If $(+, -)$ were identical with (\uparrow, \uparrow) , $\Gamma_{+-, \mu\nu}$ would very simply be $\delta_{+\mu} \delta_{-\nu}$ and the only equation of interest would be:

$$\begin{aligned}\omega \chi_{+-}(p) &= \{E_{-}(p) - E_{+}(p+Q)\} \chi_{+-}(p) \\ &\quad - \{f_{+}(p+Q) - f_{-}(p)\} \sum_{p'} \chi_{+-}(p')\end{aligned}$$

But $(+, -)$ are not identical with (\uparrow, \downarrow) and, for example,

$$a_{\uparrow}^{\dagger}(k) = \cos\left(\frac{\vec{k} \cdot \vec{a}}{\Delta}\right) a_{+}^{\dagger}(k) + \sin\left(\frac{\vec{k} \cdot \vec{a}}{\Delta}\right) a_{-}^{\dagger}(k)$$

The interaction Hamiltonian $\sum_{kk'q} a_{\uparrow}^{\dagger}(k+q) a_{\uparrow}(k) a_{\downarrow}^{\dagger}(k'+q) a_{\downarrow}(k)$

written in the $(+, -)$ representation is not of the same form as in the (\uparrow, \downarrow) representation, but is rather a complicated object which contains 2^4 terms representing all the mixtures of $+$ and $-$ in the original (\uparrow, \downarrow) operators. It can be conveniently written:

$$U \sum_{kk'q} \Lambda_{\uparrow\alpha}(k+q) a_{\alpha}^{\dagger}(k+q) a_{\beta}(k) \Lambda_{\beta\uparrow}^T(k) \times \\ \Lambda_{\downarrow\gamma}(k'-q) a_{\gamma}^{\dagger}(k'-q) a_{\delta}(k') \Lambda_{\delta\downarrow}^T(k')$$

The matrix $\Lambda(k)$ which transforms between the $(+, -)$ and (\uparrow, \downarrow) representations is

$$\Lambda(k) = \begin{pmatrix} \cos\left(\frac{\vec{k} \cdot \vec{a}}{\Delta}\right) & \sin\left(\frac{\vec{k} \cdot \vec{a}}{\Delta}\right) \\ -\sin\left(\frac{\vec{k} \cdot \vec{a}}{\Delta}\right) & \cos\left(\frac{\vec{k} \cdot \vec{a}}{\Delta}\right) \end{pmatrix}$$

Terms in the Hamiltonian which come from the off-diagonal terms of $\Lambda(k)$ give rise to coupling among susceptibilities of different spin indices. The easiest way just to see how the mixing comes about is to think of the equivalent variational calculation described previously. There is now a term in H proportional to, for example, $a_{+}^{\dagger} a_{+} a_{+}^{\dagger} a_{-}$, and this has a matrix element between excitations $a_{-}^{\dagger} a_{+}$ and $a_{+}^{\dagger} a_{+}$. Precisely the analogous thing occurs in the equations of motion for the susceptibilities.

The details of the calculation of the equations of motion are given in Appendix 1. These equations are:

$$\begin{aligned}
\omega \chi_{+-} &= \{E_-(p) - E_+(p+Q)\} \chi_{+-} \\
&- \{f_+(p+Q) - f_-(p)\} \sum_{p'} \left\{ 1 - \frac{\{(p-p') \cdot a\}^2}{\Delta^2} - \frac{(Q \cdot a)^2}{\Delta^2} \right\} \chi_{+-}(p') \\
&- \{f_+(p+Q) - f_-(p)\} \sum_{p'} \frac{(p'-p+Q) \cdot a}{\Delta} \chi_{--}(p') \\
&+ \{f_+(p+Q) - f_-(p)\} \sum_{p'} \frac{(p'-p-Q) \cdot a}{\Delta} \chi_{++}(p')
\end{aligned}$$

$$\begin{aligned}
\omega \chi_{++} &= \{E_+(p) - E_+(p+Q)\} \chi_{++} \\
&+ \{f_+(p+Q) - f_+(p)\} \sum_{p'} \frac{(p-p'-Q) \cdot a}{\Delta} \chi_{+-}(p') \\
&+ \{f_+(p+Q) - f_+(p)\} \sum_{p'} \chi_{--}(p')
\end{aligned}$$

$$\begin{aligned}
\omega \chi_{--} &= \{E_-(p) - E_-(p+Q)\} \chi_{--} \\
&+ \{f_-(p+Q) - f_-(p)\} \sum_{p'} \frac{(p'-p-Q) \cdot a}{\Delta} \chi_{+-}(p') \\
&+ \{f_-(p+Q) - f_-(p)\} \sum_{p'} \chi_{++}(p')
\end{aligned}$$

It will prove useful to represent these equations in the very schematic form:

$$\chi_{\alpha\beta}(p) = \frac{\Gamma_{\alpha\beta,\mu\nu} \chi_{\mu\nu}(p')}{D_{\alpha\beta}}$$

$D_{\alpha\beta}$ is the energy difference $\{\omega - E_\beta(p) + E_\alpha(p+Q)\}$; $\Gamma_{\alpha\beta,\mu\nu}$ is a function of \vec{p} and another momentum \vec{p}' . The variable \vec{p}' is understood to be summed over, as are repeated spin indices.

We must now consider the problem of the density fluctuations. The short range interaction $U \sum_i n_{i\uparrow} n_{i\downarrow}$ really has its origin in the long range Coulomb interaction which gives rise to the plasmon. The plasmon

dominates in the susceptibility $\chi_{++} + \chi_{--}$ and, we claim, suppresses the mixing of this susceptibility with χ_{+-} . The inclusion of a long range potential in the Hamiltonian would suppress the interaction of the density fluctuations with the spin wave, but it would also lead to great complications in solving these coupled equations of motion. It is not known exactly how to treat the long range potential in this way. We can, however, suppress the density fluctuations explicitly.

At present we have, in the (\uparrow, \downarrow) frame of reference, four equations of motion for $\chi_{\uparrow\downarrow}$, $\chi_{\downarrow\uparrow}$, $\chi_0 = \chi_\rho \equiv \frac{1}{2}(\chi_{\uparrow\uparrow} + \chi_{\downarrow\downarrow})$ and $\chi_m \equiv \frac{1}{2}(\chi_{\uparrow\uparrow} - \chi_{\downarrow\downarrow}) = \chi_z$. More succinctly, we have equations for four quantities χ^i , where $\chi_{ab} = \chi^i \sigma_{ab}^i$ and the σ^i are the three Pauli matrices and the unit matrix. We shall insist that the terms which have been omitted from our equations because the long potential has been omitted from H have the effect of suppressing χ_0 . Removing χ_0 from the equations will lead to a slight modification of the matrix elements $\Gamma_{\alpha\beta, \mu\nu}$.

Let us begin with the equations of motion in the $(+, -)$ representation in the schematic form given above:

$$\chi_{\alpha\beta}(p) = \frac{\Gamma_{\alpha\beta, \mu\nu}}{D_{\alpha\beta}} \chi_{\mu\nu}(p')$$

Since $\chi_{\alpha\beta}(p) = \langle\langle a_\alpha^\dagger(p+Q) a_\beta(p); S_-(-Q) \rangle\rangle^R$ and we know how to transform $a(p)$'s with the matrices $\Lambda(p)$, we can easily write a corresponding equation of motion in the (\uparrow, \downarrow) representation. (The convention will be that Roman letters signify that the indices are \uparrow or \downarrow , Greek signify $+$ or $-$.)

Such an equation of motion is

$$\chi_{ab}(p) = \Lambda_{a\alpha}^T(p+Q) \frac{\Gamma_{\alpha\beta,\mu\nu}}{D_{\alpha\beta}} \Lambda_{\beta b}(p) \Lambda_{\mu m}(p'+Q) \chi_{mn}(p') \Lambda_{nv}^T(p')$$

Now we define $\chi_{ab} = \chi^i \sigma_{ab}^i$ and write three equations for $\chi^{1,2,3}$ from which χ^0 has been eliminated. These are, for $m = 1, 2, 3$:

$$\chi^m = \frac{1}{2} \sum_{j=1}^3 \Lambda_{\beta b}(p) \sigma_{ba}^m \Lambda_{a\alpha}^T(p+Q) \frac{\Gamma_{\alpha\beta,\mu\nu}}{D_{\alpha\beta}} \Lambda_{\mu m}(p'+Q) \chi^j \sigma_{mn}^j \Lambda_{nv}^T(p')$$

If we transform these equations back to the (+, -) representation, the equations of motion become:

$$\begin{aligned} \chi_{\alpha\beta}(p) &= \frac{1}{2} \sum_{i,j=1}^3 \Lambda_{\alpha a}(p+Q) \Lambda_{\beta' b'}(p) \sigma_{ab}^i \sigma_{b'a'}^i \Lambda_{b\beta'}^T(p) \\ &\quad \Lambda_{\alpha' a'}^T(p+Q) \frac{\Gamma_{\alpha' \beta', \mu\nu}}{D_{\alpha\beta}} \Lambda_{\mu m}(p'+Q) \chi^i \sigma_{mn}^i \Lambda_{nv}^T(p') \end{aligned}$$

Defining

$$\tilde{\chi}_{\alpha\beta} = \chi_{\alpha\beta} - \{ \Lambda(p'+Q) \Lambda^T(p') \}_{\alpha\beta} \{ \Lambda^T(p'+Q) \Lambda(p') \}_{\mu'\nu'} \frac{1}{2} \chi_{\mu'\nu'}$$

we find

$$\tilde{\chi}_{\alpha\beta} = \left\{ \frac{\Gamma_{\alpha\beta,\mu\nu}}{D_{\alpha\beta}} - \frac{1}{2} \{ \Lambda(p+Q) \Lambda^T(p) \}_{\alpha\beta} \{ \Lambda(p+Q) \Lambda^T(p) \}_{\alpha'\beta'} \frac{\Gamma_{\alpha'\beta',\mu\nu}}{D_{\alpha'\beta'}} \right\}$$

It is useful to make one last redefinition,

$$\chi_{\alpha\beta} \equiv \frac{\Gamma_{\alpha\beta,\mu\nu}}{D_{\alpha\beta}} \tilde{\chi}_{\alpha\beta}$$

then

$$D_{\alpha\beta} \chi_{\alpha\beta} = \Gamma_{\alpha\beta,\mu\nu} \left\{ \chi_{\mu\nu} - \frac{1}{2} \{ \Lambda(p+Q) \Lambda^T(p) \}_{\mu\nu} \{ \Lambda(p+Q) \Lambda^T(p) \}_{\mu'\nu'} \chi_{\mu'\nu'} \right\}$$

and this is the modified equation of motion. The matrix $\Lambda \Lambda^T$ is very simple in form:

$$\Lambda \Lambda^T = \begin{pmatrix} \cos \frac{\vec{Q} \cdot \vec{a}}{\Delta} & -\sin \frac{\vec{Q} \cdot \vec{a}}{\Delta} \\ \sin \frac{\vec{Q} \cdot \vec{a}}{\Delta} & \cos \frac{\vec{Q} \cdot \vec{a}}{\Delta} \end{pmatrix}$$

Then, to order a^2 , the equations of motion become:

$$\begin{aligned} \omega \chi_{+-} &= \{E_-(p) - E_+(p+Q)\} \chi_{+-} \\ &- \{f_+(p+Q) - f_-(p)\} \sum_{p'} \left[1 - \frac{\{(p-p') \cdot a\}^2}{\Delta^2} - \frac{1}{2} \frac{(Q \cdot a)^2}{\Delta^2} \right] \chi_{+-}(p') \\ &- \{f_+(p+Q) - f_-(p)\} \sum_{p'} \frac{(p' - p + \frac{1}{2}Q) \cdot a}{\Delta} \chi_{--}(p') \\ &+ \{f_+(p+Q) - f_-(p)\} \sum_{p'} \frac{(p' - p - \frac{1}{2}Q) \cdot a}{\Delta} \chi_{++}(p') \end{aligned}$$

$$\begin{aligned} \omega \chi_{++} &= \{E_+(p) - E_+(p+Q)\} \chi_{++} \\ &+ \{f_+(p+Q) - f_-(p)\} \sum_{p'} \frac{(p - p' - \frac{1}{2}Q) \cdot a}{\Delta} \chi_{+-}(p') \end{aligned}$$

$$\begin{aligned} \omega \chi_{--} &= \{E_-(p) - E_-(p+Q)\} \chi_{--} \\ &+ \{f_-(p+Q) - f_-(p)\} \sum_{p'} \frac{(p' - p - \frac{1}{2}Q) \cdot a}{\Delta} \chi_{+-}(p') \end{aligned}$$

These differ from the original equations only very slightly; only the manner in which \vec{Q} appears in the matrix elements $\Gamma_{\alpha\beta, \mu\nu}$ has changed.

The secular equation for the spin wave frequency is now obtained by directly substituting the expressions for χ_{++} and χ_{--} into the χ_{+-} equation. Then an approximate solution for χ_{+-} :

$$\chi_{+-}(p) = - \frac{f_+(p+Q) - f_-(p)}{D_{+-}(p)} \sum_{p'} \chi_{+-}(p')$$

is inserted in the \vec{p}' sums which are already explicitly of order a^2 .

Summing over momenta \vec{p} , we find the secular equation:

$$\begin{aligned}
 1 &= U \sum_{\vec{p}} \frac{f_+(p+Q) - f_-(p)}{E_-(p) - E_+(p+Q) - \omega} \\
 &- U \sum_{\vec{p}, \vec{p}'} \frac{f_+(p+Q) - f_-(p)}{E_-(p) - E_+(p+Q) - \omega} \frac{f_+(p'+Q) - f_-(p')}{E_-(p') - E_+(p'+Q) - \omega} \left[\frac{(\vec{p}-\vec{p}' \cdot \vec{a})^2}{\Delta^2} + \frac{(\vec{Q} \cdot \vec{a})^2}{2\Delta^2} \right] \\
 &- \lim_{\tau \rightarrow \infty} U \sum_{\vec{p}'} \frac{f_-(p'+Q) - f_+(p')}{\omega - E_-(p') + E_-(p'+Q) + i/\tau} \left[U \sum_{\vec{p}} \frac{f_-(\vec{p}+Q) - f_+(\vec{p})}{E_-(\vec{p}) - E_-(\vec{p}+Q) - \omega_0} \frac{(\vec{p}-\vec{p}-\frac{1}{2}\vec{Q}) \cdot \vec{a}}{\Delta} \right]^2 \\
 &- \lim_{\tau \rightarrow \infty} U \sum_{\vec{p}'} \frac{f_+(p+Q) - f_+(p)}{\omega - E_+(p) + E_+(p+Q) + i/\tau} \left[U \sum_{\vec{p}} \frac{f_-(\vec{p}+Q) - f_+(\vec{p})}{E_-(\vec{p}) - E_-(\vec{p}+Q) - \omega_0} \frac{(\vec{p}-\vec{p}+\frac{1}{2}\vec{Q}) \cdot \vec{a}}{\Delta} \right]^2
 \end{aligned}$$

The evaluation of the shift in the spin wave stiffness now becomes a question of fortitude. The denominators $\{E_-(p) - E_+(p+Q) - \omega\}$ can be expanded in powers of $1/\Delta$ and all the integrations carried out to order $Q^2 a^2$.

Consider first the unperturbed secular equation:

$$1 = U \sum_{\vec{p}} \frac{f_+(p+Q) - f_-(p)}{E_-(p) - E_+(p+Q) - \omega}$$

If the occupations and energies are the ordinary Stoner ground state occupations and energies, this is the usual secular equation with $\omega = DQ^2$ as a solution. However, the energies $E_{\pm}(p)$ contain terms proportional to $(\vec{p} \cdot \vec{a})^2/\Delta$; and the occupations are Fermi functions of the perturbed energies. In the strong limit there is an $O(a^2)$ shift in the chemical potential necessary to keep the number equal to its Stoner ground state value; in the weak limit there is another $O(a^2)$ shift in chemical potential which comes about because of the

repopulation of the spin states. Each of these make a contribution to ω proportional to $Q^2 a^2$ or $(Q \cdot a)^2$.

The perturbation terms explicitly proportional to a^2 are relatively simple. Because they are already proportional to a^2 , the integrals can be evaluated using the Stoner ground state occupations; and basically ω is just proportional to the sum of these integrals. The last two terms are integrations over the + and - spin Fermi surfaces with denominators that do not contain the gap Δ . That is, the denominators may vanish, giving the integral some imaginary part: the spin wave thus can decay into an excitation of the type $a_{\sigma}^{\dagger}(p+Q) a_{\sigma}(p) |\Phi_0\rangle$, a single spin particle hole pair.

The evaluation of the change in Δ is presented in Appendix 2. It has been done for the strong limit and parabolic bands: the shift could also be evaluated fairly easily in the weak limit for parabolic bands if that were of interest. The parabolic band approximation is really an unrealistic description of nickel. It has been used because it is the only way to extract some information from these otherwise very complicated integrals. Hence any numerical result of such a calculation cannot be taken too seriously. We want rather to have a good idea of the order of magnitude of the shift in the stiffness and an understanding of its origin and structure.

We find that

$$\begin{aligned} \omega = & D_0 Q^2 - 2D_0 a^2 - \frac{3}{4p_F^2} \{ (Q \cdot a)^2 - Q^2 a^2 \} 4D_0^2 - \frac{3}{4p_F^2} (Q \cdot a)^2 \\ & + \frac{3(Q \cdot a)^2}{2\Delta} + Q^2 a^2 \left(\frac{p_F^2}{3\Delta^2} - \frac{6p_F^4}{35\Delta^3} \right) + (Q \cdot a)^2 \left(\frac{66p_F^4}{175\Delta^3} - \frac{6p_F^2}{5\Delta^2} \right) \end{aligned}$$

The inverse lifetime due to scattering with the spin conserving

excitations $a_{\sigma}^{\dagger}(p+Q) a_{\sigma}(p) |\Phi_0\rangle$ is $1/\tau = \frac{3\pi D_0 Q^2}{4p_F Q} \frac{(\vec{a} \times \vec{Q})^2}{Q^2}$.

The shift in D is, in part, similar to the result of Izuyama. In particular, the terms of order $1/\Delta^3$ are identical to his, and the terms of order $1/\Delta^2$ are similar. The terms proportional to $1/\epsilon_F$ do not appear in a calculation that does not take account of the spin wave scattering from the single particle excitations.

In the strong limit this calculation gives a positive coefficient for the $T^{5/2}$ term of the spin wave stiffness. The spin wave stiffness is expected to decrease with temperature and in fact it does, because of the temperature dependence of the usual RPA expression for D . In parabolic bands

$$D_0 = \frac{1}{2} - \frac{(\hat{Q} \cdot k)^2}{\Delta} (T)$$

and D_0 has a temperature dependence

$$= \frac{1}{3\Delta} \frac{3}{5} \frac{N\mu_0}{N} \frac{5\pi^2}{12} \frac{(kT)^2}{\mu_0^2}$$

We wish now to make a numerical estimate for the effect of the background on the spin wave stiffness. Let us first perform the angular average over the momenta of the background fluctuations. Then, including both of these temperature dependent contributions to the stiffness:

$$D = D_0 - D_1 T^2 + D_2 \overline{a^2}$$

The average of the background a^2 will give a $T^{5/2}$ temperature dependence:

$$D = D_0 (1 - D_1 T^2 + D_2 T^{5/2})$$

In the approximation of parabolic bands for nickel, a strong ferromagnet, we can now make an estimate for the coefficients D_1 and D_2 .

We need to know the parameters: $m = 5.5 m_e$; $\Delta = 0.4$ eV; $\mu = 0.27$ eV;

$n_+ - n_- = 0.6 \times$ number of atoms; number of atoms/volume $= 9.14 \times 10^{22} \text{ cm}^{-3}$.

Then we estimate $D_1 = 0.8 \times 10^{-6}$ and $D_2 = 1.0 \times 10^{-9}$. This can be compared to the result of Izuyama's formulation, $D_2(\text{Izuyama}) = 6 \times 10^{-9}$.^[11] As order of magnitude estimates, these are both in accord with the only experimental values available, which come from spin wave resonance experiments.

A numerical estimate for the lifetime is similarly,

$$1/\tau = 0.75 \times 10^{-9} \text{ eV } \overset{\circ}{\text{A}} \text{ } Q \text{ } T^{5/2}$$

The term $-2Da^2$ of ω comes as something of a surprise, as it seems to violate rotational invariance. The spin wave creation operator for $\vec{Q} = 0$ should simply rotate the whole system and hence should have no energy change associated with it. The interpretation of this term is the subject of the next section.

III Spin Wave Dispersion Relation and Rotational Invariance

We make two claims about the term $-2Da^2$ in the spin wave frequency ω : First, in the Fermi liquid case of independent spin waves, when we are trying to compute the interaction energy of two single spin waves and ω is certainly expected to have a rotationally invariant form, ω does in fact have such a form in the fixed frame of reference; the term $-2Da^2$ is cancelled by an explicit time dependence of the creation and annihilation operators which we have not yet taken into account. Second, the appearance of such a Q -independent term in ω is nevertheless a real physical effect, when we are dealing with background fluctuations of large amplitude. The spin wave creation operator at $Q = 0$ does not rotate the spins about

a fixed axis, but about a locally determined axis. Hence even at $Q = 0$, the spin wave creation operator makes a differential rotation and in general has some energy associated with it.

Before we discuss the time dependence of the collective excitation, we should examine the time dependence of the spinors themselves.

Recall that the \uparrow spinor is defined as
$$e^{-ib/2} \begin{pmatrix} \cos(\theta/2)e^{-i\phi/2} \\ \sin(\theta/2)e^{+i\phi/2} \end{pmatrix}.$$

The phases ϕ and b have been understood to be the time independent quantities $\vec{q} \cdot \vec{r}$ and $\vec{q} \cdot \vec{r} \cos\theta$ respectively. Such a magnetization configuration cannot be time independent, however; the phase ϕ is in reality $\vec{q} \cdot \vec{r} - \alpha t$. α is to be determined by the Landau-Lifshitz equation

$$\frac{\partial \vec{M}}{\partial t} = -D \vec{M} \times \nabla^2 \vec{M}$$

For $\vec{\nabla} M_z = 0$ and $\vec{\nabla} M_{\pm} = \pm i \vec{\nabla} \phi \sin\theta e^{\pm i\phi} = i \vec{\nabla} \phi M_{\pm}$

these equations are $\partial\theta/\partial t = 0$

$$\sin\theta \partial\phi/\partial t = -\sin\theta \cos\theta D (\nabla\phi)^2.$$

Then $\phi = \vec{q} \cdot \vec{r} - \alpha t$, with $\alpha = D \cos\theta q^2$.

Now for the Fermi liquid case, where θ is constant and small, it makes sense to look at the collective excitation in the fixed frame of reference; and it is the frequency of the excitation in this frame which should be in accord with the general form required to give rotational invariance of the energy. The wave function of the excitation is

$$e^{-i\omega(Q)t} \left\{ \sum_p c_p a_{-}^{\dagger}(p+Q) a_{+}(p) + u_p a_{+}^{\dagger}(p+Q) a_{+}(p) \right\}$$

Now to transform to the fixed frame of reference, we need

$$\begin{aligned}
a_{\uparrow}(k) &= \cos(\theta/2) e^{-i(\dot{b}+\dot{\phi})t/2} a_{+1}(k-q_1) \\
&\quad + \sin(\theta/2) e^{-i(\dot{b}-\dot{\phi})t/2} a_{-1}(k-q_2) \\
a_{\downarrow}(k) &= \cos(\theta/2) e^{+i(\dot{b}+\dot{\phi})t/2} a_{-1}(k+q_1) \\
&\quad - \sin(\theta/2) e^{+i(\dot{b}-\dot{\phi})t/2} a_{+1}(k+q_2)
\end{aligned}$$

We have defined $\vec{q}_1 = \vec{q}(1 - \cos\theta)/2$

and $\vec{q}_2 = \vec{q}(1 + \cos\theta)/2$

To lowest order in q and θ , the excitation in the fixed frame is:

$$\begin{aligned}
&e^{-i\omega(Q)t} \sum_p c_p(Q) e^{-i(\dot{b}+\dot{\phi})t} a_{-1}^{\dagger}(p+Q+q_1) a_{+1}(p-q_1) \\
&= e^{-i(\omega(Q)+\dot{b}+\dot{\phi})t} \sum_p c_{p+q_1}(Q) a_{-1}^{\dagger}(p+Q+2q_1) a_{+1}(p)
\end{aligned}$$

In the fixed frame, one sees an excitation of momentum \vec{Q}' and $\omega(Q')$ with a dispersion relation:

$$\omega(Q') = \omega_o(Q) + 2Da^2.$$

That is, in the fixed frame, to order θ^2

$$\begin{aligned}
\omega(Q) &= D_o(Q-2q_1)^2 - 2D_o a^2 + BQ^2 a^2 + C(\vec{Q} \cdot \vec{a})^2 + 2D_o a^2 \\
&= D_o Q^2 - 2\vec{Q} \cdot \vec{q} \sin^2\theta/2 + BQ^2 a^2 + C(\vec{Q} \cdot \vec{a})^2
\end{aligned}$$

The term $-2Da^2$ has disappeared, but the Fermi liquid coefficients B and C are unchanged. The term $-2\vec{q} \cdot \vec{Q} \sin^2\theta/2$ is not ruled out by the requirement of rotational invariance. The frequency must take a rotationally invariant form only after an isotropic average of the background \vec{q} 's is performed; after this average is done, any term proportional to $\vec{q} \cdot \vec{Q}$ will disappear.

Next, we would like to show that such a term nevertheless is in general a real physical effect and that it has its origin in the

non-linearity of the equations of motion for the magnetization. We shall solve the Landau-Lifshitz equation for a small amplitude excitation which is superimposed on a fluctuating background. Then in the frame of reference determined by the Euler angles $\theta(r)$, $\phi(r)$, and $b(r)$, the magnetization has a time dependence $e^{i\Omega t}$ with $\Omega = \omega(Q) - 2D_0 a^2$. Simply to demonstrate that such a term appears in Ω , it suffices to examine the simplest possible case, which is that of θ constant and small.

Let $\vec{M} = \vec{M}_0 + \vec{M}'$; \vec{M}_0 being itself a solution of the Landau-Lifshitz equation and representing the fluctuating background. \vec{M}_0 is to be described by θ , $\phi = \vec{q} \cdot \vec{r} - \omega t$, $\omega = D_0 q^2$. Then the Landau-Lifshitz equation is approximately

$$\frac{\partial \vec{M}'}{\partial t} = -D_0 \{ \vec{M}' \times \nabla^2 \vec{M}_0 + \vec{M}_0 \times \nabla^2 \vec{M}' \}$$

Using the explicit solution for \vec{M}_0

$$\frac{\partial M'_z}{\partial t} = -\frac{iD_0}{2} \sin\theta \{ e^{-i\phi} (q^2 + \nabla^2) M'_+ - e^{i\phi} (q^2 + \nabla^2) M'_- \}$$

$$\frac{\partial M'_+}{\partial t} = -D_0 \{ i q^2 \sin\theta e^{i\phi} M'_z - i \cos\theta \nabla^2 M'_+ + i \sin\theta e^{i\phi} \nabla^2 M'_z \}$$

Taking for a solution $M'_+ = e^{i\phi} A_+$, the equations become:

$$\frac{\partial A_+}{\partial t} = i D_0 \cos\theta (\nabla^2 + i \vec{q} \cdot \vec{\nabla}) A_+ - i \sin\theta (Q^2 + \nabla^2) M_z$$

$$\frac{\partial M_z}{\partial t} = \frac{i}{2} \sin\theta D_0 \{ (\nabla^2 + 2i \vec{q} \cdot \vec{\nabla}) A_+ + \text{complex conjugate} \}$$

At $\cos\theta = 1$, a solution is $A_+ = e^{i\phi} = e^{i\vec{Q} \cdot \vec{r} - \Omega_0 t}$ with $\frac{\Omega_0}{D_0} = Q^2 + 2\vec{q} \cdot \vec{Q}$.

For $\cos\theta \neq 1$, we can find an approximate solution by treating $\sin\theta$

as a perturbation. We take $A_+ = e^{i\phi'} + i\alpha \sin \phi_0$ and $\phi' = Q \cdot r - (\Omega_0 + \delta\Omega)t$. α and $\delta\Omega$ are to be determined, and are proportional at least to $\sin\theta$.

The M_z equation is now $-\partial M_z / \partial t = \sin\theta \Omega_0 \sin\phi$; and $M_z = \cos\phi_0 \sin\theta$. The real and imaginary parts of the A_+ equation determine α and Ω , to give:

$$\Omega_0 + \delta\Omega = Q^2 + 2q \cdot Q - \sin^2\theta q \cdot Q - \sin^2\phi q^2/2.$$

Now we wish to examine the phase of M_+ as seen in the frame of reference given by angles ϕ , b , and θ . M' is a rather complicated object. However, it consists of some wave $e^{i\phi'}$ plus other terms proportional to $\sin^2\theta$, so it will be sufficient to examine the term proportional to one. Now M_+ is simply $e^{i\phi} e^{i\phi'} \equiv e^{i(Q' \cdot r - \omega(Q')t)}$. \vec{Q}' is easily seen to be $\vec{Q} - \vec{q} \cos\theta$ and

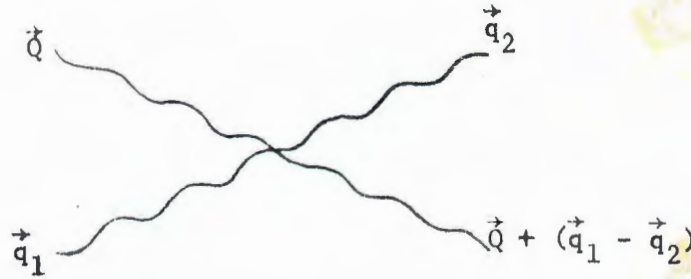
$$\omega(Q') = D_0 Q'^2 - 2D_0 a^2.$$

Thus the appearance of this form of the energy in the expression for the energy in the rotated frame is a natural consequence of the non-linearity of the equations of motion.

CHAPTER 4

SPIN WAVE-SPIN WAVE SCATTERING

In this chapter we treat the random magnetic vector potential which has up to now been ignored. As opposed to the effect of \vec{A} on the spin wave treated in the last chapter, taking account of \vec{A} does not have an effect on the Fermi liquid parameters, because \vec{A} is zero unless there are present in the system at least two distinct spin waves of wavevectors \vec{q}_1 and \vec{q}_2 not in the same direction. If we now impose a shorter wavelength excitation \vec{Q} on the system, the random magnetic field will lead to a spin wave lifetime resulting from the following spin wave-spin wave scattering:



It will first be of interest to calculate the effective vector potential for the case of a background consisting of precisely two spin waves \vec{q}_1 and \vec{q}_2 . Recall that \vec{A} is

$$\int \frac{d^3 r'}{4\pi |r-r'|} \quad \vec{\nabla}_r \times (\vec{\nabla}_{r'} \cos \theta \times \vec{\nabla}_{r'} \phi)$$

We create a two-spin wave state by making two successive rotations of the magnetization with the rotation operators associated with the spin waves \vec{q}_1 and \vec{q}_2 . These rotations tilt the angle θ by the small

amount $\theta_0 = 2/M$ and rotate about the z-axis by $\phi_1 = \vec{q}_1 \cdot \vec{r}$. To find the angles $\theta(r)$ and $\phi(r)$ we examine the spinor produced by these two successive rotations. Such a resultant spinor is to order θ_0

$$\uparrow = \begin{pmatrix} 1 \\ \frac{1}{2} \sin \theta_0 (e^{i\phi_1} + e^{i\phi_2}) \end{pmatrix} \equiv \begin{pmatrix} 1 \\ \sin \frac{1}{2} \theta e^{i\phi} \end{pmatrix}$$

The angle $\phi = \tan^{-1} \left(\frac{\sin \phi_1 + \sin \phi_2}{\cos \phi_1 + \cos \phi_2} \right)$

and $\vec{\nabla} \phi = \frac{1}{2} (\vec{q}_1 + \vec{q}_2)$

Similarly, $\sin \frac{1}{2} \theta = \frac{1}{2} \sin \theta_0 \{ (\sin \phi_1 + \sin \phi_2)^2 + (\cos \phi_1 + \cos \phi_2)^2 \}^{\frac{1}{2}}$,
giving $\vec{\nabla} \cos \theta = \theta_0^2 \sin(\phi_1 - \phi_2) (\vec{q}_1 - \vec{q}_2)$

Then $\vec{A}(r) = \frac{\vec{q} \times (\vec{q} \times \vec{Q}')}{q^2} \cos(\vec{q} \cdot \vec{r}) \equiv \vec{A}_0 \cos(\vec{q} \cdot \vec{r})$

defining \vec{q} as $(\vec{q}_1 - \vec{q}_2)$ and \vec{Q}' as $\frac{1}{2}(\vec{q}_1 + \vec{q}_2)$. Thus $\vec{A} = 0$ unless \vec{q}_1 and \vec{q}_2 are distinct. In general, θ_0^2 can be replaced by $\theta_1 \cdot \theta_2$.

Now we would like to find the effect of such a vector potential on the spin wave lifetime, treating \vec{A} independently of \vec{a} , which was treated in the last chapter.

The method for finding the contribution to the spin wave lifetime is precisely that used in Chapter 3: we look for a pole in the transverse susceptibility χ_{+-} . Since it is \vec{a} that mixes the spins parallel and anti-parallel to the local magnetization direction to make new spin eigenstates, we need not worry about which spin representation we should use. On the other hand, the vector potential has caused us to lose translational invariance, so that we must work with a more general susceptibility:

$$\chi(q, Q) \equiv \langle\langle S_+(q); S_-(-Q) \rangle\rangle$$

with \vec{q} not necessarily equal to \vec{Q} . Again we write equations of motion for the susceptibility $\chi_{+-}(Q, Q)$, ignoring the inhomogeneous terms,

$$\chi_{+-}(Q, Q) = \langle\langle [S_+(Q), H]; S_-(-Q) \rangle\rangle ;$$

and we find equations for χ by making a Hartree-Fock approximation on the right hand side.

The vector potential term of the Hamiltonian

$$\begin{aligned} H = & \sum_{k\sigma} n(k, \sigma) \varepsilon(k) + \sum_{kk'} H_{kk'}(A) \sigma a_{\sigma}^{\dagger}(k) a_{\sigma}(k') \\ & + U \sum_{kk'\lambda} a_{\uparrow}^{\dagger}(k+\lambda) a_{\uparrow}(k) a_{\downarrow}^{\dagger}(k'-\lambda) a_{\downarrow}(k') \\ H_{kk'} = & -\frac{1}{2}(k \cdot A_0) \{ \delta(k - k', q) + \delta(k - k', -q) \} \end{aligned}$$

has two effects. First, $H_{kk'}$ mixes $\chi(Q, -Q)$ with $\chi(Q + q, Q)$ and $\chi(Q - q, Q)$. Second, when we make the Hartree-Fock approximation we have $\langle a_{\sigma}^{\dagger}(k_1) a_{\sigma}(k_2) \rangle$ and this is no longer simply $\delta(k_1, k_2) f_{\sigma}(k_1)$, because these Bloch states are no longer eigenstates of the Hamiltonian; the Green's function has been modified by \vec{A} also. This too will result in mixing of $\chi(Q, Q)$ and $\chi(Q \pm q, -Q)$. The mixing of susceptibilities in these equations of motion then gives rise to a perturbation of the spin wave frequency ω as it did in the previous chapter.

II Modification of the Green's Function

We shall want to know the modification of $\langle a_{\sigma}^{\dagger}(k) a_{\sigma}(k') \rangle$ when we do the Hartree-Fock approximation. Any change which makes $\vec{k} \neq \vec{k}'$ will also couple the susceptibility $\chi(Q, Q)$ to $\chi(Q \pm q, Q)$ and so such a change should be calculated to order $|\vec{A}|$ only. A change in $\langle a_{\sigma}^{\dagger}(k) a_{\sigma}(k') \rangle$ proportional to $\delta(k - k')$ should be calculated to order A^2 .

$\langle a^{\dagger}(k) a(k') \rangle$ can be written as the Green's function $G(k, t; k', t+\epsilon)$ and Fourier transformed

$$\langle a^{\dagger}(k) a(k') \rangle = \int \frac{d\omega}{2\pi} e^{i\omega\epsilon} G(k, k', \omega)$$

Such an expression is useful, because it is known in the theory of superconductivity how to treat the effect of a weak magnetic field $\vec{\nabla} \times \vec{A}$ on this Green's function. An approximate Green's function can be shown to be^[12]

$$G(r, r', \omega) = e^{i\Phi(r, r')} G_0(r, r', \omega) .$$

G_0 is the Green's function in the absence of the magnetic field, and $\Phi(r, r')$ is

$$\Phi(r, r') = \frac{e}{2c} \{ \vec{A}(r) + \vec{A}(r') \} \cdot (\vec{r} - \vec{r}') .$$

For our situation, this quantity is $\{ \cos(\vec{q} \cdot \vec{r}) + \cos(\vec{q} \cdot \vec{r}') \} \vec{A}_0 \cdot (\vec{r} - \vec{r}') / 2$.

Therefore

$$\langle a^{\dagger}(k) a(k') \rangle = \int \frac{d\omega}{2\pi} e^{-i\omega\epsilon} \int d^3r d^3r' \exp\{ik \cdot r - ik' \cdot r' + \Phi(r, r')\} G_0(r - r', \omega)$$

We expand $\exp\{i\Phi(r, r')\}$ in powers of $|A|$ and calculate $\langle a^{\dagger}(k) a(k') \rangle$ to the appropriate order in $|A|$.

The first correction to the usual value $\delta(k - k') f(k)$ is

$$\int \frac{d\omega}{2\pi} e^{-i\omega\epsilon} \int d^3R d^3r \frac{i\vec{A}_0 \cdot \vec{r}}{2} G_0(r, \omega) \{ \cos \vec{q} \cdot (\vec{R} + \frac{\vec{r}}{2}) + \cos \vec{q} \cdot (\vec{R} - \frac{\vec{r}}{2}) \} e^{ik \cdot (\vec{R} + \frac{\vec{r}}{2})} \times \\ \exp\{ik' \cdot (\vec{R} - \frac{\vec{r}}{2})\}$$

The integration over the variable $\vec{R} = (\vec{r} + \vec{r}')/2$ gives the delta functions

$$\int \frac{d\omega}{2\pi} e^{-i\omega\epsilon} \vec{A} \cdot \vec{\nabla}_k \int d^3r \cos(\vec{q} \cdot \vec{r}/2) \{ \delta(k - k' + q) + \delta(k - k' - q) \} \times \\ G_0(r, \omega) \exp\{i(\vec{k} + \vec{k}') \cdot \vec{r}/2\}$$

The $\cos(\vec{q} \cdot \vec{r}/2)$ can now be dropped, since it merely displaces the Green's function by $\pm \vec{q}$ and the modification is already computed here to order $|A|$. Hence this term is

$$\{ \delta(k - k' - q) + \delta(k - k' + q) \} \vec{A} \cdot \vec{\nabla}_k f(k)$$

The second term in the expansion of the exponential is similarly treated. This gives

$$\int \frac{d\omega}{2} e^{-i\omega\epsilon} \int d^3R d^3r \left(\frac{i\vec{A} \cdot \vec{r}}{8} \right)^2 e^{i\vec{k} \cdot (\vec{R} + \frac{\vec{r}}{2})} - i\vec{k} \cdot (\vec{R} - \frac{\vec{r}}{2}) G_0(r, \omega) \{ \cos \vec{q} \cdot (\vec{R} + \frac{\vec{r}}{2}) + \\ \cos \vec{q} \cdot (\vec{R} - \frac{\vec{r}}{2}) \}^2$$

This is proportional to $|A|^2$ and so we are only interested in the part of this proportional to $\delta(k - k')$. Again, a $\cos(\vec{q} \cdot \vec{r}/2)$ merely displaces the value of \vec{k} at which the Green's function is evaluated and so to correct order can be replaced by 1. Then this second order term is $\delta(k - k') (\vec{A} \cdot \vec{\nabla}_k)^2 f(k)$.

The modified expectation of $a^\dagger(k) a(k')$ is hence

$$\langle a^\dagger(k) a(k') \rangle = \delta(k - k') \{ f(k) + (A \cdot \nabla)^2 f(k) \} \\ + \{ \delta(k - k' - q) + \delta(k - k' + q) \} \vec{A} \cdot \vec{\nabla} f(k)$$

It should be noted that these changes in the distribution, though they will affect the equations of motion, do not change the numbers of particles of either spin, that is, they do not change the magnetization.

III Equation of Motion for the Susceptibility $\chi_{+-}(\tilde{q}, Q)$

We are now prepared to treat the equation of motion for the general susceptibility $\chi(\tilde{q}, Q)$:

$$\chi(p; \tilde{q}, Q) = \langle\langle [a_{\sigma}^{\dagger}(p + \tilde{q}) a_{\sigma}(p), H]; S_{-}(-Q) \rangle\rangle.$$

The commutator with the single particle Hamiltonian

$$\sum_{k\sigma} \epsilon(k) n(k, \sigma) + \sum_{kk'} H_{kk'} a_{\sigma}^{\dagger}(k) a_{\sigma}(k')$$

is very simple in form. As usual, it gives a difference between the energy at \vec{p} and the energy at $\vec{p} + \vec{q}$. The term $H_{kk'}$ does the same, except that since it is zero except for $\vec{k} = \vec{k}' \pm \vec{q}$, it mixes the susceptibility $\chi(p; \tilde{q}, Q)$ with $\chi(p; \tilde{q} \pm q, Q)$. Hence the single particle contribution to the right hand side is:

$$\begin{aligned} & \{\epsilon(p) - \epsilon(p + \tilde{q})\} \chi(p; \tilde{q}, Q) + \vec{p} \cdot \vec{A}_0 \chi(p + q; \tilde{q} - q, Q) \\ & + (\vec{p} + \vec{\tilde{q}}) \cdot \vec{A}_0 \chi(p; \tilde{q} + q, Q) + (\vec{p} + \vec{\tilde{q}}) \cdot \vec{A}_0 \chi(p; \tilde{q} - q, Q) \\ & + \vec{p} \cdot \vec{A}_0 \chi(p - q, \tilde{q} + q, Q) \end{aligned}$$

To second order in the wavevectors \vec{q}_1 and \vec{q}_2 this is

$$\begin{aligned} & \{\epsilon(p) - \epsilon(p + \tilde{q})\} \chi(p; \tilde{q}, Q) + \vec{A}_0 \cdot (2\vec{p} + \vec{\tilde{q}}) \chi(p; \tilde{q} - q, Q) \\ & + \vec{A}_0 \cdot (2\vec{p} + \vec{\tilde{q}}) \chi(p, \tilde{q} + q, Q) \end{aligned}$$

In the terms coming from the commutator with the two-particle Hamiltonian we feel the effect of the modification of the Green's function. This commutator makes a contribution to the right hand side of the equation of motion:

$$\begin{aligned} & U \sum_{kk'} \{ \langle a_{+}^{\dagger}(k) a_{+}(k') \rangle - \langle a_{-}^{\dagger}(k) a_{-}(k') \rangle \} \chi(p; \tilde{q} + k - k', Q) \\ & - U \sum_{p' \lambda} \{ \langle a_{+}^{\dagger}(p + \tilde{q} + \lambda) a_{+}(p + \tilde{q}) \rangle - \langle a_{-}^{\dagger}(p + \lambda) a_{-}(p) \rangle \} \chi(p'; \tilde{q} - \lambda, Q) \end{aligned}$$

As we noted above, the modification of the Green's function does not

change the magnetization; therefore, the first term is the usual spin band gap term of the energy difference $\{E_-(p) - E_+(p + \tilde{q})\}$. The second term leads to an additional coupling of $\chi(Q, Q)$ with $\chi(Q \pm q, Q)$.

The equation of motion is now:

$$\begin{aligned} \{\omega - \varepsilon(p) + \varepsilon(p + \tilde{q}) - \Delta\} \chi(p; \tilde{q}, Q) = & \\ & \left(-U \{f_+(p + \tilde{q}) - f_-(p)\} \right. \\ & \left. + (\vec{A} \cdot \vec{\nabla})^2 f_+(p + \tilde{q}) - (\vec{A} \cdot \vec{\nabla})^2 f_-(p) \right) \sum_{p'} \chi(p', \tilde{q}, Q) \\ & + \vec{A}_0 \cdot (2\vec{p} + \vec{\tilde{q}}) \chi(p; \tilde{q} - q, Q) + \vec{A}_0 \cdot (2\vec{p} + \vec{\tilde{q}}) \chi(p; \tilde{q} + q, Q) \\ & + \{U\vec{A} \cdot \vec{\nabla} f_+(p + \tilde{q}) + U\vec{A} \cdot \vec{\nabla} f_-(p)\} \sum_{p'} \{ \chi(p; \tilde{q} + q, Q) + \chi(p; \tilde{q} - q, Q) \} \end{aligned}$$

Now we can particularize these to equations of motion for $\chi(p; Q, Q)$ and the two susceptibilities with which it mixes, $\chi(p; Q + q, Q)$ and $\chi(p; Q - q, Q)$. To simplify the notation, let us define

$$\begin{aligned} \chi(0) &\equiv \sum_{p'} \chi(p'; Q, Q) \equiv \sum_{p'} \chi(p', 0) \\ \chi(q) &\equiv \sum_{p'} \chi(p'; Q + q, Q) \equiv \sum_{p'} \chi(p', q) \end{aligned}$$

Then the equations are:

$$\begin{aligned} \{\omega - \varepsilon(p) + \varepsilon(p + Q + q) - \Delta\} \chi(p, q) = & \\ & -U \{f_+(p + Q) - f_-(p)\} \chi(q) \\ & + U (\vec{A}_0 \cdot \vec{\nabla} f_+ + \vec{A}_0 \cdot \vec{\nabla} f_-) \chi(0) + \vec{A}_0 \cdot (2\vec{p} + \vec{Q}) \chi(p, 0) \end{aligned}$$

and

$$\begin{aligned} \{\omega - \varepsilon(p) + \varepsilon(p + Q) - \Delta\} \chi(p, 0) = & -U \{f_+(p + Q) - f_-(p)\} \chi(0) \\ & + U (\vec{A}_0 \cdot \vec{\nabla} f_+ + \vec{A}_0 \cdot \vec{\nabla} f_-) \{\chi(q) + \chi(-q)\} \\ & + \vec{A}_0 \cdot (2\vec{p} + \vec{Q}) \chi(p, q) + \vec{A}_0 \cdot (2\vec{p} + \vec{Q}) \chi(p, -q) \end{aligned}$$

Define

$$Y_0(q) \equiv \sum_p \frac{f_+(p+Q+q) - f_-(p)}{\omega - \varepsilon(p) + \varepsilon(p+Q+q) - \Delta}$$

and note that

$$1 + UY_0(q) = D(q+Q)^2 - \omega$$

Then $\chi(p, q)$ has a solution

$$\frac{\vec{A}_0 \cdot (2\vec{p} + \vec{Q}) \chi(p, 0) + U(\vec{A}_0 \cdot \vec{\nabla} f_+ + \vec{A}_0 \cdot \vec{\nabla} f_-) \chi(0)}{\omega - \varepsilon(p) + \varepsilon(p+Q) - \Delta} + \frac{1}{1 + UY_0(q)} \frac{\{f_+(p+Q) - f_-(p)\}U}{\omega - \varepsilon(p) + \varepsilon(p+Q) - \Delta} \int d^3p' \frac{\vec{A}_0 \cdot (2\vec{p}' + \vec{Q}) \chi(p', 0) + U(\vec{A}_0 \cdot \vec{\nabla} f_+ + \vec{A}_0 \cdot \vec{\nabla} f_-) \chi(0)}{\omega - \varepsilon(p') + \varepsilon(p'+Q) - \Delta}$$

This can be inserted into the equation for $\chi(p, 0)$ to give:

$$\begin{aligned} \{\omega - \varepsilon(p) + \varepsilon(p+Q) - \Delta\} \chi(p, 0) &= -U\{f_+(p+Q) - f_-(p)\} \chi(0) \\ &+ \frac{2U(\vec{A}_0 \cdot \vec{\nabla} f_+ + \vec{A}_0 \cdot \vec{\nabla} f_-)}{1 + UY_0(q)} \int d^3p' \frac{\vec{A}_0 \cdot (2\vec{p}' + \vec{Q}) \chi(p', 0) + U(\vec{A}_0 \cdot \vec{\nabla} f_+ + \vec{A}_0 \cdot \vec{\nabla} f_-) \chi(0)}{\omega - \varepsilon(p') + \varepsilon(p'+Q) - \Delta} \\ &+ 2\vec{A}_0 \cdot (2\vec{p} + \vec{Q}) \left(\frac{\vec{A}_0 \cdot (2\vec{p} + \vec{Q}) \chi(p, 0) + U(\vec{A}_0 \cdot \vec{\nabla} f_+ + \vec{A}_0 \cdot \vec{\nabla} f_-) \chi(0)}{\omega - \varepsilon(p) + \varepsilon(p+Q) - \Delta} \right) \\ &+ \frac{2U\{f_+(p+Q) - f_-(p)\} \vec{A}_0 \cdot (2\vec{p} + \vec{Q})}{\{1 + UY_0(q)\} \{\omega - \varepsilon(p) + \varepsilon(p+Q) - \Delta\}} \times \\ &\times \int \frac{\vec{A}_0 \cdot (2\vec{p}' + \vec{Q}) \chi(p', 0) + U(\vec{A}_0 \cdot \vec{\nabla} f_+ + \vec{A}_0 \cdot \vec{\nabla} f_-) \chi(0)}{\omega - \varepsilon(p') + \varepsilon(p'+Q) - \Delta} d^3p' \end{aligned}$$

The secular equation is now found by taking an approximate solution:

$$\chi(p, 0) = \frac{-U\{f_+(p+Q) - f_-(p)\} \chi(0)}{\omega - \varepsilon(p) + \varepsilon(p+Q) - \Delta} ;$$

$$\omega \approx DQ^2$$

and integrating on the variable \vec{p} . This gives:

$$\begin{aligned}
 1 &= U \int \frac{f_+(p+Q) - f_-(p)}{\omega - \epsilon(p) + \epsilon(p+Q) - \Delta} d^3p \\
 &+ 2U \int d^3p \frac{\vec{A}_0 \cdot (2\vec{p} + \vec{Q})}{\{\omega - \epsilon(p) + \epsilon(p+Q) - \Delta\}^2} \left[U(\vec{A}_0 \cdot \vec{\nabla} f_+ + \vec{A}_0 \cdot \vec{\nabla} f_-) - \frac{\vec{A}_0 \cdot (2\vec{p} + \vec{Q}) \{f_+(p+Q) - f_-(p)\}}{\omega - \epsilon(p) + \epsilon(p+Q) - \Delta} \right] \\
 &+ \frac{2}{1 + UY_0(q)} \left[\int d^3p \left(\frac{-\vec{A}_0 \cdot (2\vec{p} + \vec{Q}) \{f_+(p+Q) - f_-(p)\}}{\{\omega - \epsilon(p) + \epsilon(p+Q) - \Delta\}^2} + \frac{U(\vec{A}_0 \cdot \vec{\nabla} f_+ + \vec{A}_0 \cdot \vec{\nabla} f_-)}{\omega - \epsilon(p) + \epsilon(p+Q) - \Delta} \right) \right]^2
 \end{aligned}$$

The integrals are easily done once again by expanding the denominators in powers of $1/\Delta$ and replacing ω by DQ^2 in the corrections to the unperturbed secular equation. Then

$$0 = \omega/\Delta - DQ^2/\Delta$$

$$\begin{aligned}
 &+ 2U \int d^3p \frac{\vec{A}_0 \cdot (2\vec{p} + \vec{Q})}{\{\omega - \epsilon(p) + \epsilon(p+Q) - \Delta\}^2} \left[U(\vec{A}_0 \cdot \vec{\nabla} f_+ + \vec{A}_0 \cdot \vec{\nabla} f_-) - \frac{\vec{A}_0 \cdot (2\vec{p} + \vec{Q}) \{f_+(p+Q) - f_-(p)\}}{\omega - \epsilon(p) + \epsilon(p+Q) - \Delta} \right] \\
 &- \lim_{\tau \rightarrow \infty} \frac{2}{DQ^2 - D(Q+q)^2 + i/\tau} \times \\
 &\times \left[\int d^3p \left(\frac{-\vec{A}_0 \cdot (2\vec{p} + \vec{Q}) \{f_+(p+Q) - f_-(p)\}}{\{\omega - \epsilon(p) + \epsilon(p+Q) - \Delta\}^2} + \frac{U(\vec{A}_0 \cdot \vec{\nabla} f_+ + \vec{A}_0 \cdot \vec{\nabla} f_-)}{\omega - \epsilon(p) + \epsilon(p+Q) - \Delta} \right) \right]^2
 \end{aligned}$$

The first integral correction to the unperturbed secular equation gives a purely real correction to the spin wave energy, proportional to $Q^2 A^2$. In principle, this correction is of the same order of magnitude as the corrections found in Chapter 3 and should be included with that result. In a Fermi liquid theory, however, where a background of a single spin is considered, this term is in any case zero, since it requires two distinct spin waves to be present in the background.

The part of the correction of interest is the imaginary part, which is an inverse lifetime. We can rewrite \vec{A}_0 in terms of the two spin waves of the background, \vec{q}_1 and \vec{q}_2 . The lifetime of the spin wave \vec{Q} is then a sum over the spin waves of the background,

$$\begin{aligned} 1/\tau = & -\text{Im} \int \frac{d^3q_1 d^3q_2}{DQ^2 - D(Q+\vec{q}_1-\vec{q}_2)^2} \{v(q_1)\{1-v(q_2)\} + v(q_2)\{1-v(q_1)\}\} \\ & \times 32D^2 \left(\vec{Q} \cdot \frac{(\vec{q}_1 - \vec{q}_2) \times \{(\vec{q}_1 - \vec{q}_2) \times \frac{1}{2}(\vec{q}_1 + \vec{q}_2)\}}{|\vec{q}_1 - \vec{q}_2|^2} \right) \end{aligned}$$

This expression for the lifetime, or for the scattering vertex proportional to

$$D_0 \cdot Q \cdot \left(\frac{(\vec{q}_1 - \vec{q}_2) \times \{(\vec{q}_1 - \vec{q}_2) \times \frac{1}{2}(\vec{q}_1 + \vec{q}_2)\}}{|\vec{q}_1 - \vec{q}_2|^2} \right)$$

is the result we have been seeking.

The reader may notice that the real part of the integral above has a leading term proportional to A^2 only, which would seem to lead to a real correction to DQ^2 which is proportional to DA^2 . In fact, no such correction is present because of a cancellation between the purely real correction to ω and the real part of the integral over the scattering vertex.

The former can easily be integrated to lowest order to give $-8DA^2$. We want to compare this to the real part of the scattering integral, and to do this an angular average of \vec{q}_1 and \vec{q}_2 must be taken. The angular average is $-8D (2/3) \frac{1}{2} \overline{(\vec{q}_1 + \vec{q}_2)^2}$. This is precisely cancelled by the leading term of the angular average of the scattering vertex. The details of the integration can be found in Appendix 3.

CHAPTER 5

SUMMARY

Let us now return our attention to the experiments which we originally set out to understand.

1) The spin band gap, as seen in de Haas-van Alphen measurements, does not decrease in proportion to the average magnetization, but much more slowly.

2) Spin waves of short wavelength propagate above T_C with a stiffness reduced only to about half its zero temperature value.

3) Even above the Curie temperature, magnetic degrees of freedom play a role in determining thermodynamic properties.

In chapter 2, we found that eigenstates in the presence of a fluctuating magnetization background are almost parallel or anti-parallel to the local magnetization direction. By transforming to the frame of the local magnetization, we take into account most of the effect of the fluctuations. The effect of the fluctuations in this frame appears only as a slight tilt of the eigenspinors away from the direction of local magnetization and as small shifts in the $+$ and $-$ spin energies. As the temperature increases and the average magnetization decreases, a population difference can still be maintained between spin split bands, the bands now being defined in terms of spin directions in or opposite to the direction of the local magnetization. The change from the zero temperature value of the average gap for vertical transitions is not proportional to the change in the macroscopic magnetization, but rather is proportional

only to a small repopulation of the spin bands. At low temperature this repopulation is only weakly dependent on temperature, being proportional to $T^{5/2}$ for an ordinary ferromagnet and exponentially small for the strong limit. At high temperature, to find the temperature dependence of the average gap, it is necessary to perform a functional integration which we are not able to evaluate. Nevertheless, our qualitative result remains that the magnetization and gap decrease as $\delta\Delta/\Delta \sim (\vec{q} \cdot \vec{v})^2/\Delta^2$ which may certainly be small even above T_C . Thus we can understand that a decrease of the spin band gap is not seen by the de Haas-van Alphen effect; we can also understand that the spin wave does not become degenerate with the Stoner continuum even at high temperature, so that a spin wave can have a long lifetime at such temperatures.

The magnetic degrees of freedom are still important in computing thermodynamic properties above T_C . We have found the free energy

$$F(M) = D \frac{|\vec{v}M|^2}{M} + \frac{(M - M_0)^2}{2\chi}$$

The free energy allows us to understand why the thermodynamic properties are Heisenberg-like near and above the critical temperature: this free energy is very similar in form to the free energy used to compute thermodynamic properties for localized models. Finally, the presence of the term $D|\vec{v}M|^2/M$ in the free energy leads to the usual Landau-Lifshitz equation of motion for the magnetization:

$$\frac{\partial \vec{M}}{\partial t} = - D \vec{M} \times \nabla^2 \vec{M}$$

It is the existence of a population difference and energy gap, rather than a macroscopic average magnetization that permits the

existence of a spin flip collective excitation. We found a secular equation for the frequency of the spin wave in the presence of fluctuations which was the same in form as the usual RPA secular equation, except that the appropriate Fermi functions and energies were those of the + and - eigenstates and except for the presence of small perturbative terms. The spin wave stiffness is relatively unchanged by the fluctuations, because the band properties are relatively unchanged.

We have obtained very general expressions for the corrections to the spin wave frequency and lifetime in terms of magnetization gradients of the background. These expressions include the effect of the perturbation of the single electron energy by the background, and also of the scattering of the spin wave from other excitations. In particular, in Chapter 3 we found a spin wave lifetime caused by scattering from single particle spin-conserving excitations. In Chapter 4, we considered the effect of the effective magnetic field, to find a vertex for the scattering of spin waves with the spin wave excitations of the background. These lifetime effects are quite small and allow for propagation even above T_C .

Thus it is a prediction of our theory that one see spin waves even above the critical temperature, so long as an appropriate population difference maintains a locally ordered magnetization. Such spin waves do not indeed have infinite lifetime, but the decay time is quite long.

APPENDIX I:

Equations of motion for dynamical susceptibility in the presence of \vec{a}

$$\chi_{+ -}(p) \equiv \langle\langle a_{+}^{\dagger}(p+Q) a_{-}(p); S^{-}(-Q) \rangle\rangle^R$$

$$\omega \chi_{+ -}(p) = \langle\langle [a_{+}^{\dagger}(p+Q) a_{-}(p), H]; S^{-}(-Q) \rangle\rangle^R$$

$$H = \sum_k E_{+}(k) a_{+}^{\dagger}(k) a_{+}(k) + E_{-}(k) a_{-}^{\dagger}(k) a_{-}(k)$$

$$+ U \sum_{kk'q} a_{\uparrow}^{\dagger}(k+q) a_{\uparrow}(k) a_{\downarrow}^{\dagger}(k'-q) a_{\downarrow}(k') + \frac{U}{2} \langle n_{\uparrow} - n_{\downarrow} \rangle \sum_k (n_{\uparrow}(k) - n_{\downarrow}(k))$$

1) The Kinetic energy commutator:

$$\sum_k [a_{+}^{\dagger}(p+Q) a_{-}(p), E_{+}(k) a_{+}^{\dagger}(k) a_{+}(k) + E_{-}(k) a_{-}^{\dagger}(k) a_{-}(k)]$$

$$= E_{-}(p+Q) a_{+}^{\dagger}(p+Q) a_{-}(p) - E_{+}(p) a_{+}^{\dagger}(p+Q) a_{-}(p)$$

and this contributes to $\omega \chi_{+ -}(p)$:

$$E_{-}(p) - E_{+}(p+Q) \chi_{+ -}(p)$$

2) Magnetic energy commutator:

Notice that these commutators are of the general form

$$\sum_{k_1 k_2 k_3} a^{\dagger}(p) a(k_1) a^{\dagger}(k_2) a(k_3) f(k_1, k_2, k_3)$$

In the Hartree-Fock approximation this provides the equation of motion with terms of two sorts:

$$\chi(p) \sum_{k_2 k_3} f(k_2, k_3) \langle a^\dagger(k_2) a(k_3) \rangle$$

$$\text{and } \langle a^\dagger(p) a(k_3) \rangle \sum_{p'} \chi(p') g(p').$$

The terms of the first sort effectively contribute another piece to the energy difference of (1): they are a Hartree-Fock energy difference.

But the Hartree-Fock approximation for $U \sum_{kk'q} a^\dagger_+(k+q) a_+(k) a^\dagger_-(k'-q) \times a_-(k')$ is subtracted away in the third term of H. Hence we need only consider terms of the second kind.

Below, I list the terms of H that contribute to the susceptibility equations to second order in \vec{a} , the value of the commutator with $a^\dagger_+(p+Q) a_-(p)$, and the Hartree-Fock contribute to the rhs of the equation of motion.

$$a) \quad H_a = U \sum_{kk'q} \cos\left(\frac{k \cdot a}{\Delta}\right) \cos\left(\frac{(k+q) \cdot a}{\Delta}\right) \cos\left(\frac{k' \cdot a}{\Delta}\right) \cos\left(\frac{(k'-q) \cdot a}{\Delta}\right) \times$$

$$a^\dagger_+(k+q) a_+(k) a^\dagger_-(k'-q) a_-(k')$$

$$[S_{+-}, H_a] = U \sum_{kk'q} \cos\left(\frac{k \cdot a}{\Delta}\right) \cos\left(\frac{(k+q) \cdot a}{\Delta}\right) \cos\left(\frac{k' \cdot a}{\Delta}\right) \cos\left(\frac{(k'-q) \cdot a}{\Delta}\right)$$

$$\{ \delta(p, k' - q) a^\dagger_+(p+Q) a^\dagger_+(k+q) a_+(k) a_-(k') \}$$

$$- \delta(k, p+Q) a^\dagger_+(k+q) a^\dagger_-(k'-q) a_-(k') a_-(p) \}$$

$$- \cos\left(\frac{(p+Q) \cdot a}{\Delta}\right) \cos\left(\frac{p \cdot a}{\Delta}\right) (f_+(p+Q) - f_-(p)) \sum_{p'} \cos\left(\frac{(p'+Q) \cdot a}{\Delta}\right) \cos\left(\frac{p' \cdot a}{\Delta}\right)$$

$$\chi_{+-}(p')$$

$$b) \quad H_b = -U \sum_{kk'q} \sin\left(\frac{k \cdot a}{\Delta}\right) \sin\left(\frac{k' \cdot a}{\Delta}\right) a_+^\dagger(k+q) a_-(k) a_-^\dagger(k'-q) a_+(k')$$

$$[S_{+-}, H_b] = U \sum_{kk'q} \sin\left(\frac{k \cdot a}{\Delta}\right) \sin\left(\frac{k' \cdot a}{\Delta}\right)$$

$$\{\delta(p, k' - q) a_+^\dagger(p+Q) a_+^\dagger(k+q) a_-(k) a_+(k')\}$$

$$- \delta(p+Q, k') a_+^\dagger(k+q) a_-(k) a_-^\dagger(k'-q) a_-(p)\}$$

$$\text{gives } - (f_+(p+Q) - f_-(p)) \sin\left(\frac{(p+Q) \cdot a}{\Delta}\right) \sum_{p'} \sin\left(\frac{p' \cdot a}{\Delta}\right) \chi_{+-}(p')$$

$$c) \quad H_c = -U \sum_{kk'q} \sin\left(\frac{(k'-q) \cdot a}{\Delta}\right) \sin\left(\frac{(k+q) \cdot a}{\Delta}\right) a_-^\dagger(k+q) a_+(k) a_+^\dagger(k'-q)$$

$$\times a_-(k')$$

$$[S_{+-}, H_c] = U \sum_{kk'q} \sin\left(\frac{(k+a) \cdot a}{\Delta}\right) \sin\left(\frac{(k'-q) \cdot a}{\Delta}\right)$$

$$\{\delta(k, p+Q) a_-^\dagger(k+q) a_+^\dagger(k'-q) a_-(k') a_-(p)\}$$

$$- \delta(p, k+q) a_+^\dagger(p+Q) a_+(k) a_+^\dagger(k'-q) a_-(k')\}$$

gives

$$- \sin\left(\frac{p \cdot a}{\Delta}\right) (f_+(p+Q) - f_-(p)) \sum_{p'} \sin\left(\frac{(p'+Q) \cdot a}{\Delta}\right) \chi_{+-}(p')$$

$$d) \quad H_d = U \sum_{kk'q} \sin\left(\frac{(k+q) \cdot a}{\Delta}\right) a_{-}^{\dagger}(k+q) a_{+}(k) a_{-}^{\dagger}(k'-q) a_{-}(k')$$

$$[S_{+-}, H_d] = U \sum_{kk'q} \sin\left(\frac{(k+q) \cdot a}{\Delta}\right)$$

$$\{\delta(p, k' - q) a_{-}^{\dagger}(k+q) a_{+}^{\dagger}(p+Q) a_{+}(k) a_{-}(k')$$

$$- \delta(p+Q, k) a_{-}^{\dagger}(k+q) a_{-}^{\dagger}(k'-q) a_{-}(k') a_{-}(p)$$

$$- \delta(p, k+a) a_{+}^{\dagger}(p+Q) a_{+}(k) a_{-}^{\dagger}(k'-q) a_{-}(k')\}$$

gives

$$- (f_{+}(p+Q) - f_{-}(p)) \sum_{p'} \sin\left(\frac{(p'-p+Q) \cdot a}{\Delta}\right) \chi_{--}(p')$$

$$e) \quad H_e = - U \sum_{kk'q} \sin\left(\frac{k' \cdot a}{\Delta}\right) a_{+}^{\dagger}(k+q) a_{+}(k) a_{-}^{\dagger}(k'-q) a_{+}(k')$$

$$[S_{+-}, H_e] = U \sum_{kk'q} \sin\left(\frac{k' \cdot a}{\Delta}\right)$$

$$\{\delta(k', p+Q) a_{+}^{\dagger}(k+q) a_{+}(k) a_{-}^{\dagger}(k'-q) a_{-}(p)$$

$$\delta(k, p+Q) a_{+}^{\dagger}(k+q) a_{-}^{\dagger}(k'-q) a_{+}(k') a_{-}(p)$$

$$\delta(p, k'-q) a_{+}^{\dagger}(k+q) a_{+}^{\dagger}(p+Q) a_{+}(k) a_{+}(k')\}$$

gives

$$(f_{+}(p+Q) - f_{-}(p)) \sum_{p'} \sin\left(\frac{(p'-p-Q) \cdot a}{\Delta}\right) \chi_{++}(p')$$

Expanding the sines and cosines, we find the equation of motion:

$$\begin{aligned}
 \omega \chi_{+-}(p) &= (E(p_-) - E_+(p+Q)) \chi_{+-}(p) \\
 &- (f_+(p+Q) - \delta_-(p)) \sum_{p'} \left(1 - \frac{((p-p') \cdot a)^2}{\Delta^2} - \frac{(Q \cdot a)^2}{\Delta^2}\right) \chi_{+-}(p') \\
 &- (f_+(p+Q) - f_-(p)) \sum_{p'} \frac{(p'-p+Q) \cdot a}{\Delta} \chi_{--}(p') \\
 &+ (f_+(p+Q) - f_-(p)) \sum_{p'} \frac{(p'-p-Q) \cdot a}{\Delta} \chi_{++}(p')
 \end{aligned}$$

In the same way we find the equations of motion for χ_{++} and χ_{--} :

$$\omega \chi_{++}(p) = \langle\langle [a_+^\dagger(p+Q) a_+(p), H]; S^-(-Q) \rangle\rangle^R$$

1) The kinetic energy commutator:

$$\begin{aligned}
 &\sum_k [a_+^\dagger(p+Q) a_+(p), E_+(k) a_+^\dagger(k) a_+(k)] \\
 &= E_+(p) a_+^\dagger(p+Q) a_+(p) - E_+(p+Q) a_+^\dagger(p+Q) a_+(p)
 \end{aligned}$$

gives

$$(E_+(p) - E_+(p+Q)) \chi_{++}(p)$$

2) Magnetic Energy commutators:

$$a) \quad H_a = -U \sum_{kk'q} \sin\left(\frac{(k'-q) \cdot a}{\Delta}\right) a_+^\dagger(k+a) a_+(k) a_+^\dagger(k'-q) a_-(k')$$

$$[S_{++} + H_a] = U \sum_{kk'q} \sin\left(\frac{(k'-q) \cdot a}{\Delta}\right)$$

$$\{\delta(p, k' - q) a_+^\dagger(k + q) a_+^\dagger(p + Q) a_+(k) a_-(k')$$

$$- \delta(k, p + Q) a_+^\dagger(k + q) a_+^\dagger(k' - q) a_+^\dagger(p) a_-(k')$$

$$- \delta(p, k + q) a_+^\dagger(p + Q) a_+(k) a_+^\dagger(k' - q) a_-(k')\}$$

gives

$$(f_+(p + Q) - f_+(p)) U \sum_{p'} \chi_{+-}(p') \sin\left(\frac{(p-p'-Q) \cdot a}{\Delta}\right)$$

$$b) \text{ to order } |\vec{a}|, H_b = U \sum_{kk'q} a_+^\dagger(k + q) a_+(k) a_-^\dagger(k' - q) a_-(k')$$

$$[S_{++} + H_b] = U \sum_{kk'q} \{\delta(k + q, p) a_+^\dagger(p + Q) a_+(k) a_-^\dagger(k' - q) a_-(k')$$

$$- \delta(k, p + Q) a_+^\dagger(k + q) a_-^\dagger(k' - q) a_-(k) a_+(p)\}$$

gives

$$(f_+(p + Q) - f_+(p)) U \sum_{p'} \chi_{--}(p')$$

The equation of motion is then

$$\omega \chi_{++}(p) = (E_+(p) - E_+(p + Q)) \chi_{++}(p)$$

$$+ (f_+(p + Q) - f_+(p)) U \sum_{p'} \frac{(p-p'-q) \cdot a}{\Delta} \chi_{+-}(p')$$

$$+ (f_+(p + Q) - f_+(p)) U \sum_{p'} \chi_{--}(p')$$

the equation of motion for $\chi_{--}(p)$ can be deduced from those for χ_{++} and χ_{+-} :

$$\omega \chi_{--}(p) = (E_{-}(p) - E_{-}(p + Q)) \chi_{--}(p)$$

$$+ (f_{-}(p + Q) - f_{-}(p)) \sum_{p'} \frac{(p' - p - Q) \cdot a}{\Delta} \chi_{+-}(p')$$

$$+ (f_{-}(p + Q) - f_{-}(p)) \sum_{p'} \chi_{++}(p')$$

APPENDIX II:

Evaluation of $\delta\omega(\vec{a})$

(1) Consider first the unperturbed secular equation:

$$1 = U \sum_p \frac{f_+(p+Q) - f_-(p)}{E_-(p) - E_+(p+Q) - \omega}$$

For parabolic bands, these energies are:

$$E_-(p) = p^2/2 + MU/2 + (\vec{p} \cdot \vec{a})^2/\Delta + a^2/2 - \overline{(\vec{p} \cdot \vec{a})^2}/\Delta$$

$$E_+(p+Q) = (p+Q)^2/2 - MU/2 - \{(\vec{p}+\vec{Q}) \cdot \vec{a}\}^2/\Delta + a^2/2 + \overline{(\vec{p} \cdot \vec{a})^2}/\Delta .$$

M is the number difference $n_+ - n_-$, which in turn is $M_0 + O(a^2)$

if we are not in the strong limit; $\overline{(\vec{p} \cdot \vec{a})^2}$ denoted an average over

the singly occupied states. Δ is defined as $(n_+ - n_-)U = (M_0 + \delta M)U$

in the case of a weak ferromagnet and Δ_0 for the strong limit.

Expanding the denominator in powers of $1/\Delta$, we find

$$\begin{aligned} 0 &= \int d^3p f_+(p) \left[\left(1 + \frac{(\vec{p} \cdot \vec{Q})^2}{\Delta}\right) - Q^2/2 + \frac{(\vec{p} \cdot \vec{Q})^2}{\Delta} - \frac{(\vec{Q} \cdot \vec{a})^2}{\Delta} + \right. \\ &\quad \left. + \frac{4(\vec{p} \cdot \vec{Q})(\vec{p} \cdot \vec{a})(\vec{Q} \cdot \vec{a})}{\Delta^2} - \frac{6(\vec{p} \cdot \vec{Q})^2}{\Delta^3} \{(\vec{p} \cdot \vec{a})^2 - \overline{(\vec{p} \cdot \vec{a})^2}\} \right] \\ &- \int d^3p f_-(p) \left[\left(1 + \frac{(\vec{p} \cdot \vec{Q})^2}{\Delta}\right) + Q^2/2 + \frac{(\vec{p} \cdot \vec{Q})^2}{\Delta} - \frac{(\vec{Q} \cdot \vec{a})^2}{\Delta} + \right. \\ &\quad \left. + \frac{4(\vec{p} \cdot \vec{Q})(\vec{p} \cdot \vec{a})(\vec{Q} \cdot \vec{a})}{\Delta^2} - \frac{6(\vec{p} \cdot \vec{Q})^2}{\Delta^3} \{(\vec{p} \cdot \vec{a})^2 - \overline{(\vec{p} \cdot \vec{a})^2}\} \right] \\ &= M\omega \left(1 + \frac{\overline{(\vec{p} \cdot \vec{Q})^2}}{\Delta}\right) - NQ^2/2 + \int d^3p \{f_+(p) - f_-(p)\} \left[\frac{(\vec{p} \cdot \vec{Q})^2}{\Delta} - \frac{(\vec{Q} \cdot \vec{a})^2}{\Delta} + \right. \\ &\quad \left. + \frac{4(\vec{p} \cdot \vec{Q})(\vec{p} \cdot \vec{a})(\vec{Q} \cdot \vec{a})}{\Delta^2} - \frac{6(\vec{p} \cdot \vec{Q})^2}{\Delta^3} \{(\vec{p} \cdot \vec{a})^2 - \overline{(\vec{p} \cdot \vec{a})^2}\} \right] \end{aligned}$$

The integrals explicitly proportional to $Q^2 a^2$ can be evaluated using the unperturbed Stoner equilibrium occupations. The other terms in zero order give the unperturbed spin wave energy $\omega = DQ^2$, but there are corrections to it from the shift in chemical potential and the change in the form of the eigenenergies as a function of \vec{p} . The shift in chemical potential can be expressed as the change necessary to keep the number constant plus the change caused by repopulation of the spin bands.

$$\delta\mu_\sigma = -\frac{\sigma p_{F\sigma}^2 a^2}{3\Delta} + \frac{\delta n_\sigma}{N_\sigma}$$

$$f_\sigma(p) = f_{o\sigma}(p) + \frac{\sigma(\vec{p}\cdot\vec{a})^2}{\Delta} - \frac{p_{F\sigma}^2 a^2}{3\Delta} - \frac{\delta n_\sigma}{N_\sigma} \delta(\epsilon - \epsilon_{F\sigma})$$

Hence from these terms we find

$$0 = (M + \delta M) \left(1 + \frac{(\vec{p}\cdot\vec{Q})^2}{\Delta}\right) - NQ^2/2 + \int d^3p \{f_{o+}(p) - f_{o-}(p)\} \frac{(\vec{p}\cdot\vec{Q})^2}{(M+\delta M)U}$$

$$+ \int d^3p \frac{(\vec{p}\cdot\vec{Q})^2}{\Delta} \delta(\epsilon - \epsilon_{F+}) \left(\frac{(\vec{p}\cdot\vec{a})^2}{\Delta} - \frac{p_{F+}^2 a^2}{\Delta} - \frac{\delta n_+}{N_+} \right)$$

$$- \int d^3p \frac{(\vec{p}\cdot\vec{Q})^2}{\Delta} \delta(\epsilon - \epsilon_{F-}) \left(-\frac{(\vec{p}\cdot\vec{a})^2}{\Delta} + \frac{p_{F-}^2 a^2}{\Delta} - \frac{\delta n_-}{N_-} \right)$$

$$DQ^2 = \left(1 + \frac{(\vec{p}\cdot\vec{Q})^2}{\Delta}\right) + \left[\oint_\mu + \oint_\mu \right] |v| d\Omega \frac{(\vec{p}\cdot\vec{Q})^2}{\Delta} \left(\frac{(\vec{p}\cdot\vec{a})^2}{\Delta} - \frac{(\vec{p}\cdot\vec{a})^2}{3\Delta} \right)$$

$$+ \frac{\delta M}{M_0} \left[DQ^2 + \frac{1}{M} \int d^3p \{f_{o+}(p) - f_{o-}(p)\} \frac{(\vec{p}\cdot\vec{Q})^2}{\Delta} - \frac{1}{2} \left[\frac{\oint_\mu^+}{N_+} + \frac{\oint_\mu^-}{N_-} \right] |v| d\Omega \frac{(\vec{p}\cdot\vec{Q})^2}{\Delta} \right]$$

$$- \frac{1}{M_0} \int d^3p \{f_{o+}(p) - f_{o-}(p)\} \left[\frac{(Q\cdot a)^2}{\Delta} - \frac{4(\vec{p}\cdot\vec{Q})(\vec{p}\cdot\vec{a})(Q\cdot\vec{a})}{\Delta^2} \right. \\ \left. + \frac{6(\vec{p}\cdot\vec{Q})^2}{\Delta^3} \{(\vec{p}\cdot\vec{a})^2 - \overline{(\vec{p}\cdot\vec{a})^2}\} \right]$$

In parabolic bands, this is a perfectly general expression for the contribution of the unperturbed secular equation; if all \vec{p}' 's are replaced by $\vec{v}(p)$, this will hold for arbitrary bands. The value of δM is that given on page 28 and is proportional to a^2 .

The integrals are easily evaluated but they give simple expressions only in the strong limit, when we set $M = 0$, $f_-(p) = 0$, and $M = N = 4\pi p_F^3/3$. Then

$$\begin{aligned} 0 = & \omega(1 + p_F^2 Q^2/5\Delta) - DQ^2 - (Q \cdot a)^2/\Delta - Q^2 p_F^2 a^2/3\Delta \\ & + Q^2 a^2 p_F^2/5\Delta^2 + 2(Q \cdot a)^2/5\Delta^2 + 4p_F^2 (Q \cdot a)^2/5\Delta^2 \\ & - 12p_F^4 Q^2 a^2/175\Delta^3 + 60p_F^4 (Q \cdot a)^2/175\Delta^3 \end{aligned}$$

(2) Next we must evaluate:

$$U \sum_{pp'} \frac{f_+(p) - f_-(p-Q)}{E_-(p-Q) - E_+(p) - \omega_0} \frac{f_+(p') - f_-(p'-Q)}{E_-(p'-Q) - E_+(p') - \omega_0} \left(\frac{(Q \cdot a)^2}{2\Delta^2} + \frac{\{(\vec{p}' - \vec{p}) \cdot \vec{a}\}^2}{\Delta^2} \right)$$

To order $Q^2 a^2$, the first term is simply $(Q \cdot a)^2/2\Delta$. To do the next, first use the symmetry of \vec{p} and \vec{p}' integrations to write the matrix element $\{(\vec{p} - \vec{p}') \cdot \vec{a}\}^2/\Delta^2$ as $\{(\vec{p}' \cdot \vec{a})^2 - 2(\vec{p}' \cdot \vec{a})(\vec{p} \cdot \vec{a})\}/\Delta^2$. Then we do the \vec{p} integration. To order Q^2 , the secular equation assures us that

$$\sum_p \frac{f_+(p) - f_-(p-Q)}{E_-(p-Q) - E_+(p) - \omega_0} = \frac{1}{U}$$

so the term $(\vec{p}' \cdot \vec{a})^2$ gives only

$$2U\Delta \sum_{p'} \frac{f_+(p') - f_-(p'-Q)}{E_-(p'-Q) - E_+(p') - \omega_0} \frac{(p' \cdot a)^2}{\Delta^2}$$

We must also do

$$U^2\Delta \sum_p \frac{f_+(p) - f_-(p-Q)}{\Delta - p \cdot Q} \left(\frac{-2(p' \cdot a)(p \cdot a)}{\Delta^2} \right)$$

and this is

$$- \frac{2(p' \cdot a)^2 U^2}{\Delta} \left(\sum_{so} \frac{(p \cdot a)(p \cdot Q)}{\Delta^2} + \frac{(Q \cdot a) n_-}{\Delta} \right)$$

Integrating this last term over p' as well, we have

$$- \frac{2}{\Delta^2} \sum_{so} \left(\frac{(p \cdot a)(p \cdot Q)}{\Delta} + (Q \cdot a) n_- \right) \frac{U^2}{\Delta}$$

Finally we return to

$$\begin{aligned} & 2U\Delta \sum_{p'} \frac{f_+(p') - f_-(p' - Q)}{E(p' - Q) - E(p') - \omega_0} \frac{(p' \cdot a)^2}{\Delta} \\ &= 2U \sum_{p'} f_+(p') \frac{(p' \cdot a)^2}{\Delta^2} \left(1 - \frac{(p' \cdot Q)^2}{\Delta^2} + \frac{Q^2}{2\Delta} - \frac{DQ^2}{\Delta} \right) \\ &\quad - 2U \sum_{p'} f_-(p') \frac{(p' \cdot a)^2}{\Delta^2} \left(1 - \frac{(p' \cdot Q)^2}{\Delta^2} - \frac{Q^2}{2\Delta} - \frac{DQ^2}{\Delta} \right) \\ &\quad - 2U \sum_{p'} f_-(p') \frac{2(p' \cdot a)(a \cdot Q) + (a \cdot Q)^2}{\Delta^2} \left(1 + \frac{(p' \cdot Q)}{\Delta} \right) \\ &= - \frac{2}{M} \sum_{p'} f_-(p') \left(\frac{2(p' \cdot a)(p' \cdot Q)(a \cdot Q)}{\Delta^2} + \frac{(a \cdot Q)^2}{\Delta} \right) \\ &\quad + \frac{2}{M} \sum_{so} \frac{(p' \cdot a)}{\Delta} + \frac{2}{M} \left(\frac{1}{M} \sum_{so} \frac{(p \cdot a)^2}{\Delta} \sum_{so} \frac{(p' \cdot a)^2}{\Delta} - \sum_{so} \frac{(p \cdot a)^2 (p \cdot Q)^2}{\Delta^2} \right) \\ &\quad + \frac{2}{M} \left(\frac{Q^2}{2} \sum_{all} \frac{(p \cdot a)^2}{\Delta^2} - \frac{NQ^2}{2M} \sum_{so} \frac{(p \cdot a)^2}{\Delta^2} \right) \end{aligned}$$

Hence the total contribution to $\delta\omega$ of this first order perturbation theory integral is:

$$\begin{aligned}
& \frac{2}{M} \sum_{\text{so}} \frac{(\mathbf{p} \cdot \mathbf{a})^2}{\Delta} + \frac{2}{M\Delta} \left[\frac{1}{M} \sum_{\text{so}} \frac{(\mathbf{p} \cdot \mathbf{a})^2}{\Delta} \sum_{\text{so}} \frac{(\mathbf{p} \cdot \mathbf{Q})^2}{\Delta} - \sum_{\text{so}} \frac{(\mathbf{p} \cdot \mathbf{a})^2 (\mathbf{p} \cdot \mathbf{Q})^2}{\Delta^2} \right] \\
& - \frac{2}{M^2 \Delta} \left(\sum_{\text{so}} \frac{(\mathbf{p} \cdot \mathbf{a})(\mathbf{p} \cdot \mathbf{Q})}{\Delta} + (\mathbf{a} \cdot \mathbf{Q}) n_- \right) + \frac{(\mathbf{Q} \cdot \mathbf{a})^2}{2\Delta} \\
& - \frac{2}{M} \left(\sum_{\mathbf{p}'} f_-(\mathbf{p}') \frac{2(\mathbf{p}' \cdot \mathbf{a})(\mathbf{p}' \cdot \mathbf{Q})(\mathbf{a} \cdot \mathbf{Q})}{\Delta^2} + \frac{(\mathbf{a} \cdot \mathbf{Q})^2}{\Delta} \right) \\
& + \frac{Q^2}{M\Delta^2} \left(\sum_{\text{all}} (\mathbf{p} \cdot \mathbf{a})^2 - \frac{N}{M} \sum_{\text{so}} (\mathbf{p} \cdot \mathbf{a})^2 \right)
\end{aligned}$$

In the strong limit this is

$$\frac{(\mathbf{Q} \cdot \mathbf{a})^2}{2\Delta} + \frac{2p_F^2 a^2}{5\Delta} - \frac{4Q^2 a^2 p_F^2}{175\Delta^3} + \frac{6(\mathbf{Q} \cdot \mathbf{a})^2 p_F^4}{175\Delta^3}$$

(3) Finally we must evaluate

$$\begin{aligned}
& \frac{1}{M} \sum_{\mathbf{p}'} \frac{f_+(\mathbf{p}' + \frac{1}{2}\mathbf{Q}) - f_+(\mathbf{p}' - \frac{1}{2}\mathbf{Q})}{DQ^2 - \mathbf{p}' \cdot \mathbf{Q} + i/\tau} \left(\sum_{\mathbf{p}''} \{f_+(\mathbf{p}'' + \mathbf{Q}) - f_-(\mathbf{p}'')\} \frac{(\mathbf{p}'' - \mathbf{p}') \cdot \mathbf{a}}{\Delta - \mathbf{p}'' \cdot \mathbf{Q}} \right)^2 \\
& \frac{1}{M} \sum_{\mathbf{p}'} \frac{f_-(\mathbf{p}' + \frac{1}{2}\mathbf{Q}) - f_-(\mathbf{p}' - \frac{1}{2}\mathbf{Q})}{DQ^2 - \mathbf{p}' \cdot \mathbf{Q} + i/\tau} \left(\sum_{\mathbf{p}''} \{f_+(\mathbf{p}'' + \mathbf{Q}) - f_-(\mathbf{p}'')\} \frac{(\mathbf{p}'' - \mathbf{p}') \cdot \mathbf{a}}{\Delta - \mathbf{p}'' \cdot \mathbf{Q}} \right)^2
\end{aligned}$$

The matrix elements, that is, the \vec{p}'' integrals, are respectively

$$\begin{aligned}
& (\vec{a} \cdot \vec{Q}) \overline{p^Z} / \Delta - (\vec{p}' \cdot \vec{a}) + (\vec{Q} \cdot \vec{a}) n_- / M \\
& \text{and} \quad (\vec{a} \cdot \vec{Q}) \overline{p^Z} / \Delta - (\vec{p}' \cdot \vec{a}) + (\vec{Q} \cdot \vec{a}) n_+ / M
\end{aligned}$$

The \mathbf{p}' integrals are carried out over the Fermi surfaces of the two spins. The leading term is

$$- \frac{1}{M} \int d^3p (\mathbf{p} \cdot \mathbf{Q}) \delta(\epsilon - \epsilon_{F+}) \frac{(\mathbf{p} \cdot \mathbf{a})}{(\mathbf{p} \cdot \mathbf{Q})} - \frac{1}{M} \int d^3p (\mathbf{p} \cdot \mathbf{Q}) \delta(\epsilon - \epsilon_{F-}) \frac{(\mathbf{p} \cdot \mathbf{a})}{(\mathbf{p} \cdot \mathbf{Q})}$$

or

$$- \frac{1}{M} \left[\oint |v| d\Omega (\vec{p} \cdot \vec{a})^2 + \oint |v| d\Omega (\vec{p} \cdot \vec{a})^2 \right]$$

Specializing once more to the case of the strong limit, the real part of the Fermi surface integral proportional to $Q^2 a^2$ is

$$- \frac{3}{4p_F^2} \{ (\vec{Q} \cdot \vec{a})^2 - Q^2 a^2 \} 4D^2 - \frac{3}{4p_F^2} (\vec{Q} \cdot \vec{a})^2$$

Now, putting all the above contributions together, the secular equation becomes, in the strong limit:

$$\begin{aligned} \omega &= D_0 Q^2 - 2D_0 a^2 \\ &- \frac{3}{4p_F^2} \{ (\vec{Q} \cdot \vec{a})^2 - Q^2 a^2 \} 4D_0 - \frac{3}{4p_F^2} (\vec{Q} \cdot \vec{a})^2 \\ &+ \frac{5}{6} \frac{(\vec{Q} \cdot \vec{a})^2}{\Delta} + Q^2 a^2 \left(\frac{p_F^2}{3\Delta^2} - \frac{6}{35} \frac{p_F^2}{\Delta^3} \right) \\ &+ (\vec{Q} \cdot \vec{a})^2 \left(\frac{66}{175} \frac{p_F^2}{\Delta^3} - \frac{6}{5} \frac{p_F^2}{\Delta^2} \right) \end{aligned}$$

(4) The imaginary part of the Fermi surface integrals gives the spin wave lifetime. To lowest order in $|Q|$, this is:

$$\begin{aligned} 1/\tau &= \frac{\pi}{M} \oint_{\epsilon_{F+}} |v| d\Omega (\vec{p} \cdot \vec{Q}) \delta(DQ^2 - \vec{p} \cdot \vec{Q}) (\vec{p} \cdot \vec{a})^2 \\ &+ \frac{\pi}{M} \oint_{\epsilon_{F-}} |v| d\Omega (\vec{p} \cdot \vec{Q}) \delta(DQ^2 - \vec{p} \cdot \vec{Q}) (\vec{p} \cdot \vec{a})^2 \end{aligned}$$

Take \hat{Q} as the \hat{z} -axis. Then $(\vec{p} \cdot \vec{a})$ averaged on the angle ϕ is

$$\frac{1}{2} p^2 \sin^2 \theta (a^2 - a_z^2) + p^2 \cos^2 \theta a_z^2.$$

Because of the delta function on θ , the term of lowest order in $|Q|$ is $\frac{1}{2} p^2 (a^2 - a_z^2)$. This gives for the imaginary part:

$$\frac{2\pi}{M} \frac{1}{2} DQ^2 \frac{(\vec{a} \times \vec{Q})^2}{Q^3} \left(\frac{1}{p_{F+}} + \frac{1}{p_{F-}} \right)$$

In the strong limit, the inverse lifetime is:

$$1/\tau = \frac{3\pi}{4p_F} D_o Q^2 \frac{(\vec{a} \times \vec{Q})^2}{Q^3} .$$

APPENDIX 3:

Integrations arising from spin wave-spin wave scattering corrections to D

We want to compare the two quantities:

$$U \int d^3p \frac{2(2p+Q) \cdot a}{(\omega - \varepsilon(p) + \varepsilon(p+Q) - \Delta)^2} \left(UA \cdot \nabla f_+ + UA \cdot \nabla f_- - \frac{A \cdot (2p+Q) \{f_+(p+Q) - f_-(p)\}}{\omega - \varepsilon(p) + \varepsilon(p+Q) - \Delta} \right)$$

and

$$\frac{32 D^2 (A_0 \cdot Q)^2}{DQ^2 - D(Q+q)^2}$$

to order A^2 .

(1) To this low order, the first integrals are very simply:

$$U \int d^3p \{f_+(p) - f_-(p)\} \frac{8(p \cdot A)}{\Delta^3} + U \int d^3p \{A \cdot \nabla f_+ + A \cdot \nabla f_-\} \frac{2p \cdot A}{\Delta^2}$$

This is
$$\frac{8\overline{p^2}}{\Delta^2} - \frac{4A^2}{\Delta} = -8DA^2/\Delta.$$

Next we take an angular average on the vectors $\vec{q} = \vec{q}_1 - \vec{q}_2$ and $Q' = \frac{1}{2}(\vec{q}_1 + \vec{q}_2)$, recalling that \vec{A}_0 was defined as $\frac{\vec{q} \times (\vec{q} \times \vec{Q}')}{q^2}$.

These angular averages leave:

$$\overline{\left(\frac{q(q \cdot Q')}{q^2} - Q' \right)^2} = - \frac{\overline{(q \cdot Q')^2}}{q^2} + \overline{Q'^2} = \frac{2}{3} Q'^2$$

(2) We next want,

$$- \int d\Omega_{Q'} d\Omega_q \frac{32D^2(Q \cdot A)^2}{DQ^2 - D(Q+q)^2}$$

The angular average on \vec{Q}' leaves an integrand:

$$- 32 \frac{Q^2}{3} \frac{D}{Q^2 - (Q+q)^2} \{Q^2 - \frac{1}{3} (Q \cdot \hat{q})^2\}$$

Let \vec{Q} define the z-axis for the Ω_q integration. The real part of the

average is

$$\frac{16}{3} DQ^2 \left(\frac{1}{2} \int_{-1}^1 \frac{dx Q^2}{qQx + \frac{1}{2}q} + \frac{1}{2} \int_{-1}^1 \frac{x^2 dx Q^2}{qQx + \frac{1}{2}q} \right)$$

and this is easily seen to be $8DQ^2/3$. Hence there is no correction to ω of order A^2 only.

APPENDIX IV: Glossary

<u>Quantity</u>		<u>Page on which defined</u>
U	effective Coulomb exchange integral	5
Δ	band gap	5, 21
M	magnetization	5, 21
N	density of states at Fermi level	6
χ	static susceptibility	6
μ	chemical potential	7
$\nu(q)$	spin wave number	8
c_p, u_p, d_p	variational parameters	9, 40
D	spin wave stiffness	9
s.o.	singly occupied states	9
$S(q)$	spin density operator	11
$Y(k)$	component of susceptibility	11
$\chi_{\alpha\beta}(q, \omega)$	spin, momentum and frequency dependent susceptibility	12
χ_o	integral found in susceptibility	12
u_k	unperturbed Bloch wave function	21
$\theta(r), \phi(r)$	angles of magnetization	21
(\uparrow, \downarrow)	spinors in magnetization frame of reference	22
\vec{a}	magnetization gradient	23
\vec{A}	effective magnetic vector potential	23
b	Euler angle	23
$(+, -)$	eigenspinors	26
$\Gamma_{\alpha\beta, \mu\nu}; D_{\alpha\beta}$	abbreviations	42

<u>Quantity</u>		<u>Page</u>
$\Lambda(k)$	transformation matrix	43
χ_i	susceptibility	45
\vec{A}_0	vector potential	56
\vec{q}_1, \vec{q}_2	magnon wave vectors	57

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